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14. ABSTRACT
This report is intended to be a historical record of activities describing the research programs of the U.S. Army Research Laboratory - Army Research Office (ARL-ARO) for fiscal year 2016 (FY16; 1 Oct 2015 through 30 Sep 2016). This report provides: (i) an overview of the mission and strategy employed to guide ARO research investments and factors affecting the implementation of that strategy, (ii) a snapshot of end-of-year statistics of basic research funding (i.e., "6.1" funding) and program proposal activity, and (iii) research trends and key annual scientific discoveries and accomplishments of the ARO scientific divisions.

15. SUBJECT TERMS
Army Research Laboratory, Army Research Office, extramural basic research, high-risk and high-payoff research, future Army

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2016
ARO
IN REVIEW

U.S. Army Research Laboratory (ARL)
U.S. Army Research Office (ARO)

P.O. Box 12211

Research Triangle Park, NC 27709-2211

ARO IN REVIEW 2016

A summary of the U.S. Army Research Office (ARO) programs
for fiscal year 2016 (FY16), including program goals, management
strategies, funding information, and key accomplishments

Kelby O. Kizer, Ph.D.
Editor

ARO IN REVIEW 2016

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CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY

This report is intended to be a single-source document describing the research programs of the U.S. Army Research Office (ARO) for fiscal year 2016 (FY16; 1 Oct 2015 through 30 Sep 2016). This report provides:

- A brief review of the strategy employed to guide ARO research investments and noteworthy issues affecting the implementation of that strategy
- Statistics regarding basic research funding (*i.e.*, "6.1" funding) and program proposal activity
- Research trends and accomplishments of the individual ARO scientific divisions

I.   ARO MISSION

The mission of ARO, as part of the U.S. Army Research Laboratory (ARL), is to execute the Army's extramural basic research program in the following disciplines: chemical sciences, computing sciences, electronics, life sciences (including social science), materials science, mathematical sciences, mechanical sciences, network sciences, and physics. The goal of this basic research is to drive scientific discoveries that will provide the Army with significant advances in operational capabilities through high-risk, high pay-off research opportunities, primarily with universities, but also with large and small businesses. ARO ensures that this research supports and drives the realization of future research relevant to all of the ARL Science and Technology (S&T) Campaigns and Essential Research Areas, and that the results of these efforts are transitioned to the Army research and development community for the pursuit of long-term technological advances for the Army.

II.   ARO STRATEGY AND FUNCTION

ARO's mission represents the most long-range Army view for changes in its technology, with system applications often 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities. ARO competitively selects and funds basic research proposals from educational institutions, nonprofit organizations, and private industry. ARO executes its mission through conduct of an aggressive basic science research program on behalf of the Army to create cutting-edge scientific discoveries and the general store of scientific knowledge that is required to develop and improve weapons systems for land force dominance. The ARO research portfolio consists principally of extramural academic research efforts consisting of single investigator efforts, university-affiliated research centers, and specially tailored outreach programs. Each program has its own objectives and set of advantages as described further in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

ARL has eight S&T Campaigns (listed in Section III-B), including an extramural basic research campaign that ARO leads. ARO supports research that will lead to new discoveries and increased understanding of the physical, engineering, and information sciences as they relate to long-term national security needs, in addition to the other seven ARL Campaigns.

The ARO strategy and programs, as part of the ARL Extramural Basic Research Campaign, are formulated in concert with the other ARL S&T Campaigns, the Research, Development and Engineering Command's (RDECOM's) Research, Development and Engineering Centers (RDECs), the Army Medical Research and Materiel Command (MRMC), the Army Corps of Engineers, and the Army Research Institute for the Behavioral

and Social Sciences. ARO programs and research areas are intimately aligned with, and fully supportive of, the research priorities set within the RDECOM Campaign Plan, the DoD Quadrennial Defense Review, the DoD Strategic Basic Research Plan, the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)] S&T Priorities, the Army S&T Master Plan, the Training and Doctrine Command (TRADOC) Army Capabilities Integration Center's Integrated S&T Lines of Effort, the TRADOC Army Warfighting Challenges, and the Assistant Secretary of the Army for Acquisition, Logistics, and Technology [ASA(ALT)] Special Focus Areas.

ARO serves the following functions in pursuit of its mission.

- Execute an integrated, balanced extramural basic research program
- Create and guide the discovery and application of novel scientific phenomena leading to leap-ahead technologies for the Army
- Drive the application of science to generate new or improved solutions to existing needs
- Accelerate research results transition to applications in all stages of the research and development cycle
- Strengthen the research infrastructures of academic, industrial, and nonprofit laboratories that support the Army
- Focus on research topics that support technologies vital to the Army's future force, combating terrorism and new emerging threats
- Leverage S&T of other defense and government laboratories, academia and industry, and organizations of our allies
- Foster training for scientists and engineers in the scientific disciplines critical to Army needs
- Actively seek creative approaches to enhance the diversity and capabilities of future U.S. research programs by enhancing education and research programs at historically black colleges and universities, and minority-serving institutions

III. IMPLEMENTING ARO STRATEGY

ARO employs multiple programs, initiatives, and investment strategies to fulfill its mission. A snapshot of the ARO research programs is provided in this section, and each program is described further in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

A. Program Snapshot

The research programs managed by ARO range from single investigator research to multidisciplinary/multi-investigator centers. A typical basic research grant within a program may provide funding for a few years, while in other programs, such as research centers affiliated with particular universities, a group of investigators may receive funding for many years to pursue novel research concepts. The programs for the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) are aimed at providing infrastructure and incentives to improve the diversity of U.S. basic research programs (see CHAPTER 2-IX). In addition to supporting the education of graduate students through basic research grants, the National Defense Science and Engineering Graduate (NDSEG) fellowship program is another mechanism through which ARO fosters the training of a highly-educated workforce skilled in DoD and Army-relevant research, which is critical for the future of the nation (see CHAPTER 2-X). ARO also has extensive programs in outreach to pre-graduate education to encourage and enable the next generation of scientists (see CHAPTER 2-XI). In addition, ARO guides the transition of basic research discoveries and advances to the appropriate applied-research and advanced-development organizations. ARO is actively engaged in speeding the transition of discovery into systems, in part through involvement in the development of topics and the management of projects in the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs (see CHAPTER 2-VIII).

B. Coordination for Program Development and Monitoring

The research programs and initiatives that compose ARO's extramural research program are formulated through ongoing and active collaborations elsewhere in ARL, including the:

- ARL S&T Campaigns, in addition to the ARL Extramural Basic Research Campaign
    - Computational Sciences Campaign
    - Materials Research Campaign
    - Sciences-for-Maneuver Campaign
    - Information Sciences Campaign
    - Sciences for Lethality-and-Protection Campaign
    - Human Sciences Campaign
    - Assessment and Analysis Campaign
- ARL Essential Research Areas (ERAs), in addition to the Discovery ERA
    - Human Agent Teaming
    - Artificial Intelligence and Machine Learning
    - Cyber and Electromagnetic Technologies for Complex Environments
    - Distributed and Cooperative Engagement in Contested Environments
    - Tactical Unit Energy Independence
    - Manipulating Physics of Failure for Robust Performance of Materials
    - Science of Manufacturing at the Point of Need
    - Accelerated Learning for a Ready and Responsive Force
- ARL Directorates:
    - Computational and Information Sciences Directorate (ARL-CISD)
    - Human Research and Engineering Directorate (ARL-HRED)
    - Sensors and Electron Devices Directorate (ARL-SEDD)
    - Survivability/Lethality Analysis Directorate (ARL-SLAD)
    - Vehicle Technology Directorate (ARL-VTD)
    - Weapons and Materials Research Directorate (ARL-WMRD)

ARO programs are also formulated through collaborations with other Federal research organizations, including:

- RDECOM's RDECs
- Army Medical Research and Materiel Command (MRMC)
- Army Corps of Engineers (ACE)
- Army Research Institute for the Behavioral and Social Sciences
- Army Training and Doctrine Command (TRADOC)

ARO's extramural research program provides foundational discoveries in support of the ARL S&T Campaign Plan. While the ARL Directorates and the RDECOM Centers are the primary users of the results of the ARO research program, ARO also supports research of interest to ACE, MRMC, other Army Commands, and DoD agencies. Coordination and monitoring of the ARO extramural program by the ARL Directorates, RDECs, and other Army laboratories ensures a highly productive and cost-effective Army research effort. The University Affiliated Research Centers (UARCs) and Multidisciplinary University Research Initiative (MURI) centers benefit from the expertise and guidance provided by the ARL Directorates, RDECs, and other DoD, academic, and industry representatives who serve on evaluation panels for each UARC.

The ARO-managed OSD research programs include the University Research Initiative (URI) programs, and the Research and Educational Program (REP) for HBCU/MIs. These programs fall under the executive oversight of the Defense Basic Research Advisory Group. This group is led by the ASD(R&E) Director for Research, representatives from the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), ARO, and ASAALT.

IV. REVIEW AND EVALUATION

The ARO Directorates, Divisions, and Programs are evaluated by a wide range of internal (Army) and external (Academic, other Government) reviews, such as the biennial ARO Division Reviews. For additional information regarding these review processes, the reader is encouraged to refer to the corresponding presentations and reports from each review (not included here).

V. ARO ORGANIZATIONAL STRUCTURE

The organizational structure of ARO mirrors the departmental structure found in many research universities. ARO's scientific divisions are aligned to a specific scientific discipline (*e.g.*, chemical sciences), and supported by the Operations Directorate (see FIGURE 1).
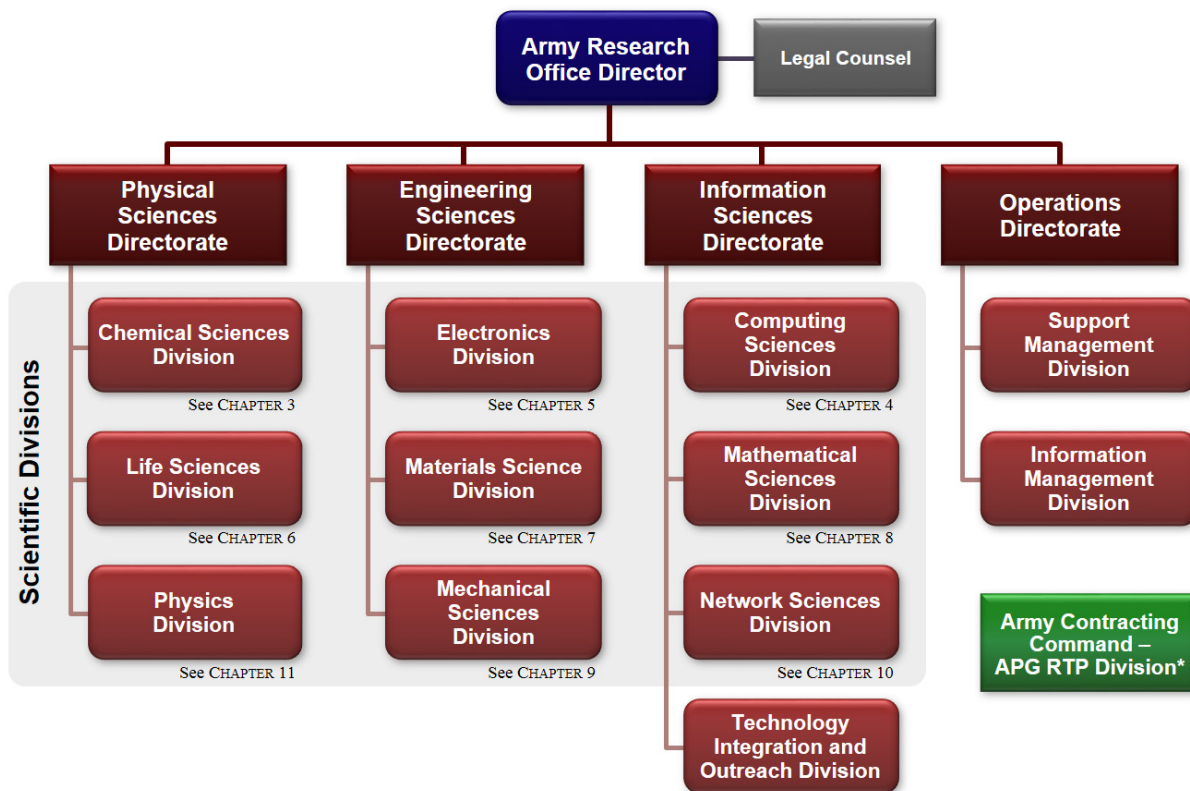
FIGURE 1

ARO Organizational Structure. ARO's scientific divisions fall under the Physical Sciences, Engineering Sciences, and Information Sciences Directorates. Each scientific Division has its own vision and research objectives, as described further in CHAPTERS 3-11. *Army Contracting Command – Army Proving Ground (APG), Research Triangle Park (RTP) Division executes the contracting needs for ARO-funded research; however, as part of the Army Contracting Command (*i.e.*, not ARL), it also performs contracting activities throughout RDECOM.

VI. ARO DIRECTOR'S OFFICE STAFF

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CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES

As described in the previous chapter, ARO pursues a variety of investment strategies to meet its mission as the Army's lead extramural basic research agency in chemical sciences, computing sciences, electronics, life sciences (including social science), materials science, mathematical sciences, mechanical sciences, network sciences, and physics. In this role, ARO serves as ARL's lead for the Extramural Basic Research Campaign (refer to CHAPTER 1 - Section III). ARO implements its investment strategies through research programs and initiatives that have unique objectives, eligibility requirements, and receive funding from a variety of DoD sources. This chapter describes the visions, objectives, and funding sources of these programs, which compose the overall ARO extramural research program.

The selection of research topics, proposal evaluation, and project monitoring are organized within ARO Divisions according to scientific discipline (refer to the organizational chart presented in CHAPTER 1). ARO's Divisions are aligned with these disciplines, each with its own vision and research objectives, as detailed in CHAPTERS 3-11. Each Division identifies topics that are included in the broad agency announcement (BAA). Researchers are encouraged to submit white papers and proposals in areas that support the Division's objectives. It is noted that the ARO Divisions are not confined to only funding research in the academic departments that align with the Division names. The Divisions have the flexibility to find and fund the most promising research to advance their mission regardless of the academic department pursuing a particular research idea.

I.   OVERVIEW OF PROGRAM FUNDING SOURCES

ARO oversees and participates in the topic generation, proposal solicitation, evaluation, and grant-monitoring activities of programs funded through a variety of DoD agencies, as listed in the following subsections.

A. Army Funding

The Army funds the majority of the extramural basic research programs managed by ARO, as listed below.
- The Core (BH57) Research Program, funded through basic research "BH57" funds (see Section II).
- The University Research Initiative (URI), which includes these component programs:
  - Multidisciplinary University Research Initiative (MURI) program (see Section III)
  - Presidential Early Career Awards for Scientists and Engineers (PECASE; see Section IV)
  - Defense University Research Instrumentation Program (DURIP; see Section V)
- Two University Affiliated Research Centers (UARCs; see Section VI)

ARO coordinates with the Office of the Secretary of Defense (OSD) in managing the URI programs and also manages the Army's Small Business Technology Transfer (STTR) program (see Section VIII).

B. Office of the Secretary of Defense (OSD) Funding

The funds for a variety of programs managed or supported by ARO are provided by OSD.
- Research and Educational Program (REP) for Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI; see Section IX)
- National Defense Science and Engineering Graduate (NDSEG) Fellowships (see Section X)
- Youth Science Activities (see Section XI)

These activities are mandated by DoD's Chief Technology Office, the Assistant Secretary of Defense for Research and Engineering ASD(R&E). Each of these OSD-funded programs has a unique focus and/or a unique target audience. ARO has been designated by ASD(R&E) as the lead agency for the implementation of REP for HBCU/MSI activities on behalf of the three Services. OSD oversees ARO management of the Army-funded URI and its component programs (MURI, PECASE, and DURIP).

C. Other Funding Sources

In addition to the Army- and OSD-funded programs described earlier in this section, ARO leverages funds from other DoD sources (*e.g.*, Defense Advanced Research Projects Agency [DARPA]) to support a variety of external programs with specific research focuses. These joint programs have objectives consistent with the strategies of the corresponding ARO Program. Due to the unique nature of these cooperative efforts, each externally-funded effort is discussed within the chapter of the aligned scientific Division (see CHAPTERS 3-11).

II. ARO CORE (BH57) RESEARCH PROGRAM

ARO's Core Research Program is funded with Army basic research "BH57" funds and represents the primary basic research funding provided to ARO by the Army. Within this program and its ongoing BAA, research proposals are sought from educational institutions, nonprofit organizations, and commercial organizations for basic research in electronics, physics, and the chemical, computing, life, materials, mathematical, mechanical, and network sciences. The goal of this program is to utilize world-class and worldwide academic expertise to discover and exploit novel scientific discoveries, primarily at universities, to provide the current and future force with critical new or enhanced capabilities.

ARO Core Research Program activities fall under five categories, discussed in the following subsections: (a) Single Investigator awards, (b) Short Term Innovative Research efforts, (c) Young Investigator Program, (d) support for conferences, workshops, and symposia, and (e) special programs. ARO's Core (BH57) Research Program represents the principal mission of ARO and is where the majority of the Army funds are used. A summary of the Core (BH57) Research Program budget is presented in Section XIII.

A. Single Investigator (SI) Program

The goal of the SI program is to pursue the most innovative, high-risk, and high-payoff ideas in basic research. Research proposals within the SI Program are received throughout the year in a continuously-open, worldwide BAA solicitation. This program focuses on basic research efforts by one or two faculty members along with supporting graduate students and/or postdoctoral researchers and is typically a three-year grant.

B. Short Term Innovative Research (STIR) Program

The objective of the STIR Program is to explore high-risk initial proof-of-concept ideas within a nine-month timeframe. Research proposals are sought from educational institutions, nonprofit organizations, or private industry. If a STIR effort's results are promising, the investigator may be encouraged to submit a proposal to be evaluated for potential longer-term funding options, such as an SI award.

C. Young Investigator Program (YIP)

The objective of the YIP is to attract outstanding young university faculty to Army-relevant research questions, to support their research, and to encourage their teaching and research careers. Outstanding YIP projects may be considered for the prestigious PECASE award (see Section IV).

D. Conferences, Workshops, and Symposia Support Program

The ARO Core Program also provides funding for organizing and facilitating scientific and technical conferences, workshops, and symposia. This program provides a method for conducting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army and help define research needs, thrusts, opportunities, and innovation.   In particular, workshops are a key mechanism ARO uses to identify new research areas with the greatest opportunities for scientific breakthroughs that will revolutionize future Army capabilities.

E. Special Programs

Although the ARO SI, STIR, YIP, and conference-support programs constitute the primary use of BH57 funds, the ARO Core Research Program also supports a variety of special programs. These special programs include matching funds applied to the ARO Core-funded HBCU/MSI program, and also the Army-supported High School Apprenticeship Program (HSAP) and Undergraduate Research Apprenticeship Program (URAP), which are part of the Youth Science Activities (see Section XI).

F. International Programs

Beginning in FY16, ARO initiated international programs with the goal of identifying academic investigators who are the forerunners in particular fields of research of which U.S. scientists do not currently hold the lead. Based on a detailed data analytics study that assessed 39 countries and their research publication output from 2009-2014, ARO identified seven scientific areas critical to the future Army, components of which are led by researchers outside of the U.S. These areas were grouped into three key geographic locations: the Atlantic, Pacific, and Americas regions.

These international programs are part of ARL and ARO's comprehensive approach to ensure that Army basic research funds are used efficiently to find the scientists best suited to drive high-risk, high-payoff Army crucial research, regardless of whether these researchers are in the U.S. or abroad. The seven ARO International Program Managers are each aligned to a particular ARO Division and focus on key research areas to identify international investigators with skills and ideas in areas not led by researchers within the U.S., as well as to engage and partner those researchers with existing Army and DoD programs. These international research areas, the corresponding aligned Division, and the locations where the International PMs are stationed are listed below.

- Energy Transport and Storage (Chemical Sciences Division) - Tokyo, Japan
- Advanced Computing (Computing Sciences Division) - São Paulo, Brazil
- Synthetic Biology (Life Sciences Division) - Tokyo, Japan
- Human Dimension (Life Sciences Division) - London, United Kingdom
- Innovation in Materials (Materials Science Division) - London, United Kingdom
- Network Science and Intelligent Systems (Network Sciences Division) - London, United Kingdom
- Quantum Scale Materials (Physics Division) - Tokyo, Japan

III. MULTIDISCIPLINARY UNIVERSITY RESEARCH INITIATIVE (MURI)

As described in Section I: *Overview of Program Funding Sources*, the MURI Program is part of the University Research Initiative (URI) and supports research teams whose research efforts intersect more than one traditional discipline. A multidisciplinary team effort can accelerate research progress in areas particularly suited to this approach by cross-fertilization of ideas, can hasten the transition of basic research findings to practical applications, and can help to train students in science and/or engineering in areas of importance to DoD.

In contrast with ARO Core program SI research projects, MURI projects support centers whose efforts require a large and highly collaborative multidisciplinary research effort. They are typically funded at $1.25 million per year for three years with an option for two additional years. These efforts are expected to enable more rapid research and development (R&D) breakthroughs and to promote eventual transition to Army applications.

Oversight of the MURI program comes from the Basic Research Office of ASD(R&E) to the Service Research Offices (OXRs), where OXR program managers (PM) manage the MURI projects. The OXRs include ARO, the Air force Office of Scientific Research (AFOSR), and the Office of Naval Research (ONR). OXR PMs have significant flexibility and discretion in how the individual projects are monitored and managed, while ASD(R&E) defends the program to higher levels in OSD and has responsibility for overall program direction and oversight. Selection of Army research topics and the eventual awards are reviewed and approved by ASD(R&E) under a formal acquisition process.

Eight MURI projects were selected for funding and began in FY16. These projects are based on proposals submitted to the FY16 MURI topic BAA, which was released in late FY14. Each new-start project, lead investigator, and lead performing organization are listed here, immediately below the corresponding MURI topic, topic authors/PMs, and the ARO Division responsible for monitoring the project. A description of each project can be found in the corresponding Division's chapter, based on the topic's lead author.

- *Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery*; PMs: Dr. Dawanne Poree (Chemical Sciences) and Dr. Stephanie McElhinny (Life Sciences)

    Project Selected: *Engineering the Translation Apparatus for the Synthesis of Electronically Active Sequence-defined Polymers*; Professor Michael Jewett, Northwestern University - Evanston

- *Discovering Hidden Phases with Electromagnetic Excitation;* PMs: Dr. Marc Ulrich (Physics) and Dr. Pani Varanasi (Materials Science)

    Project Selected: *Quantum Materials by Design with Electromagnetic Excitation*; Professor David Hsieh, California Institute of Technology

- *Modeling and Analysis of Multisensory Neural Information Processing for Direct Brain-Computer Comms*; PMs: Dr. Liyi Dai (Computing Sciences) and Dr. Frederick Gregory (Life Sciences)

    Project Selected: *Closed-Loop Multisensory Brain-Computer Interface for Enhanced Decision Accuracy*; Professor Maryam Shanechi, University of Southern California

- *Modular Quantum Systems*; PMs: Dr. T.R. Govindan (Physics) and Dr. T. Curcic (AFOSR)

    Project Selected: *Scaling Modular and Reconfigurable Quantum Systems*; Professor Christopher Monroe, Department of Physics, University of Maryland - College Park

- *Spin Textures and Dynamics Induced by Spin-Orbit Coupling*; PMs: Dr. Joe Qiu (Electronics), Dr. John Prater (Materials Science), and Dr. Marc Ulrich (Physics)

    Project Selected: *Magnetoelectrics and Spinorbitronics in Topological Heterostructures and Superlattices*; Professor Kang Wang, University of California - Los Angeles

- *Defining Expertise by Discovering the Underlying Neural Mechanisms of Skill Learning*; PMs: Dr. Frederick Gregory (Life Sciences) and Dr. Virginia Pasour (Mathematics)

    Project Selected: *Neural Foundations of Expertise Based on Optimal Decision-making, Physical Control and Responses to Stress*; Professor Scott Grafton, University of California - Santa Barbara

- *Media Analytics for Developing & Testing Theories of Social Structure and Interaction*; PMs: Dr. Purush Iyer (Network Science) and Dr. Lisa Troyer (Life Sciences)

    Project Selected: *SCAN: Socio-Cultural Attitudinal Networks*; Professor V. S. Subrahmanian, University of Maryland - College Park

- F*undamental Properties of Energy Flow and Partitioning at Sub-nanoscale Interfaces*; PMs: Dr. Robert Mantz (Chemical Sciences) and Dr. Ralph Anthenien (Mechanical Sciences)

    Project Selected: *Multi-modal Energy Flow at Atomically Engineered Interfaces*; Professor Jon-Paul Maria, North Carolina State University

The following topics were published in FY16 and constitute the ARO portion of the FY17 MURI BAA.

- *Additive 3D Self-Assembly of Responsive Materials*
    PMs: Dr. John Prater (Materials Science) and Dr. Dawanne Poree (Chemical Sciences)

- *Anyons in 2D materials and Cold Atomic Gases*
  PMs: Dr. Paul Baker and Dr. Marc Ulrich (Physics)

- *Information Content in Data for Multimodal Data Analysis*
  PM: Dr. Liyi Dai (Computing Sciences)

- *Nutritional and Environmental Effects on the Gut Microbiome and Cognition*
  PMs: Dr. Frederick Gregory and Dr. Bob Kokoska (Life Sciences)

- *Spectral Decomposition and Control of Strongly Coupled Nonlinear Interacting Systems*
  PMs: Dr. Samuel Stanton and Dr. Matthew Munson (Mechanical Sciences)

- *Toward Room Temperature Exciton-Polaritonics*
  PMs: Dr. Michael Gerhold (Electronics) and Dr. Marc Ulrich (Physics)

- *Cyber Deception through Active Manipulation of Adversaries' Cognition Process*
  PMs: Dr. Cliff Wang (Computing Sciences) and Dr. Lisa Troyer (Life Sciences)

IV. PRESIDENTIAL EARLY CAREER AWARD FOR SCIENTISTS AND ENGINEERS (PECASE)

The PECASE program, also part of the URI program, attracts outstanding young university faculty members, supporting their research, and encouraging their teaching and research careers. PECASE awards are the highest honor bestowed by the Army to extramural scientists and engineers beginning their independent research careers. Each award averages $200K/year for five years. PECASE awards are based in part on two important criteria: (i) innovative research at the frontiers of science and technology that is relevant to the mission of the sponsoring agency, and (ii) community service demonstrated through scientific leadership, education, and outreach.

The PECASE winners for each calendar year's competition are announced by the White House. The winners of the 2014 PECASE competition were announced in FY16. Of the candidates nominated by ARO, four investigators were selected to receive PECASE awards. These awards began as "new start" projects in FY16 and are listed in this section, with the project title followed by the principal investigator (PI), performing organization, ARO PM and corresponding scientific division.   Additional details for each of these projects can be found in the corresponding scientific division's chapter.

- *Synthesis and Fundamental Studies of Atomic Layers, Atomic Quilts, and van der Waals Heterostructures*
  PI: Professor Deji Akinwande, University of Texas - Austin
  ARO PM: Dr. Chakrapani Varanasi, Materials Science

- *Governmentality and Social Capital in Tribal/Federal Relations Regarding Heritage Consultation*
  PI: Professor Sarah Cowie, University of Nevada - Reno
  ARO PM: Dr. Lisa Troyer, Life Sciences

- *Ab Initio Design Of Noncentrosymmetric Metals: Crystal Engineering In Oxide Heterostructures*
  PI: Professor James Rondinelli, Drexel University
  ARO PM: Dr. Marc Ulrich, Physics

- *Weakly Supervised Learning for Scalable Semantic Parsing*
  PI: Professor Luke Zettlemoyer, University of Washington
  ARO PM: Dr. Purush Iyer, Network Sciences

V. DEFENSE UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM (DURIP)

DURIP, also part of the URI program, supports the purchase of state-of-the-art equipment that augments current university capabilities or develops new capabilities to perform cutting-edge defense research. DURIP meets a critical need by enabling university researchers to purchase equipment costing $50K or more to conduct DoD-relevant research. In FY16, the Army awarded 61 grants at $12,118,204 total, with an average award of $227K.

VI. UNIVERSITY AFFILIATED RESEARCH CENTERS (UARCs)

The University Affiliated Research Centers (UARCs) are strategic DoD-established research organizations at universities. The UARCs were formally established in May 1996 by ASD(R&E) in order to advance DoD long-term goals by pursuing leading-edge basic research and to maintain core competencies in specific domains unique to each UARC, for the benefit of DoD. One DoD Agency is formally designated by ASD(R&E) to be the primary sponsor for each UARC. The primary sponsor ensures DoD UARC management policies and procedures are properly implemented. Collaborations among UARCs and the educational and research resources available at the associated universities can enhance each UARC's ability to meet the long-term goals of DoD. ARO is the primary sponsor for two UARCs, with involvement in a third.

- The Army's Institute for Soldier Nanotechnologies (AISN), located at the Massachusetts Institute of Technology (MIT). The AISN is discussed further in CHAPTER 3: CHEMICAL SCIENCES DIVISION.
- The Army's Institute for Collaborative Biotechnologies (AICB), located at the University of California - Santa Barbara, with academic partners at MIT and the California Institute of Technology. The AICB is discussed further in CHAPTER 6: LIFE SCIENCES DIVISION.
- The Army's Institute for Creative Technologies (AICT), located at the University of Southern California. In contrast to the AISN and AICB, the AICT is co-managed within ARL by both ARO and the Human Research and Engineering Directorate (HRED). Funding for the AICT is managed through ARO while HRED provides technical guidance with ARO support.

VII. MINERVA RESEARCH INITIATIVE (MRI)

The Minerva Research Initiative (MRI) is a DoD-sponsored, university-based social science basic research program initiated by the Secretary of Defense and focuses on areas of strategic importance to U.S. national security policy. It seeks to increase the intellectual capital in the social sciences and improve DoD's ability to address future challenges and build bridges between DoD and the social science community. Minerva brings together universities, research institutions, and individual scholars and supports multidisciplinary and cross-institutional projects addressing specific topic areas determined by DoD.

Minerva projects are funded up to a five-year base period, with awards ranging from small, single investigator grants for 2-3 years to large multidisciplinary projects for $1-2 million per year for 5 years. The program is tri-service managed, with ARO managing 2-5 year projects dealing with causes and consequences of regime change, development of new models to pinpoint sources and effects of protest movements, relationships between natural disasters and sociopolitical instability, identification of demographic factors contributing to rise of global violent extremist organizations. ARO also provides scientific, technical, and managerial support to OSD in formulating the overall program.

The management of the OSD MRI program transitioned to the ARO Life Sciences division beginning in FY16. Due in part to this transition, there were no FY16 new-start MRI projects; however, new start projects are planned to begin in FY17.

VIII. SMALL BUSINESS INNOVATION RESEARCH (SBIR) AND SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAMS

Congress established SBIR and STTR programs in 1982 and 1992, respectively, to provide small businesses and research institutions with opportunities to participate in government-sponsored R&D. The DoD SBIR and STTR programs are overseen and administered by the Office of Small Business Programs within the Office of the Under Secretary of Defense for Acquisition, Technology and Logistics. The Army-wide SBIR Program is managed by RDECOM, while the Army-wide STTR Program is managed by ARO.

A. Purpose and Mission

The purpose of the SBIR and STTR programs is to (i) stimulate technological innovation, (ii) use small business to meet Federal R&D needs, (iii) foster and encourage participation by socially and economically disadvantaged small business concerns (SBCs), in technological innovation, and (iv) increase private sector commercialization of innovations derived from Federal R&D, thereby increasing competition, productivity, and economic growth. The STTR program has the additional requirement that small companies must partner with universities, federally funded research and development centers, or other non-profit research institutions to work collaboratively to develop and transition ideas from the laboratory to the marketplace.

B. Three-phase Process

The SBIR and STTR programs use a three-phase process, reflecting the high degree of technical risk involved in funding research, and developing and commercializing cutting edge technologies. The basic parameters of this three-phase process for both programs within the Army are shown in TABLE 1.

TABLE 1

Three-phase process of the SBIR and STTR programs. Phase I is an assessment of technical merit and feasibility, Phase II is a larger R&D effort often resulting in a deliverable prototype, and Phase III is a project derived from, extending, or logically concluding prior SBIR/STTR work, generally to develop a viable product or service for military or commercial markets.

	SBIR Contract Limits	**STTR Contract Limits**
Phase I	• 6 months, $100K max • 3-month option (at Government's discretion), $50K max, to fund interim Phase II efforts	• 6 months, $150K max • No options
Phase II	• 2 years, $1 million max	• 2 years, $1 million max
Phase III	• No time or size limit • No SBIR/STTR set-aside funds	• No time or size limit • No SBIR/STTR set-aside funds

1. Phase I. Phase I of the SBIR and STTR programs involves a feasibility study that determines the scientific, technical, and commercial merit and feasibility of a concept. Each SBIR and STTR BAA contains topics seeking specific solutions to stated government needs. Phase I proposals must respond to a specific topic in the BAA, and proposals are competitively judged on the basis of scientific, technical, and commercial merit. The Phase I evaluation and award process marks the entry point to the program and cannot be bypassed.

2. Phase II. Phase II represents a major research and development effort, culminating in a well-defined deliverable prototype (*i.e.*, a technology, product, or service). The Phase II selection process is also competitive. Phase I contractors can submit Phase II proposals during one of the respective program's submissions cycles, as there are no separate Phase II BAAs. Typically 50% of Phase II proposals are selected for award. SBIR Phase II awardees may be selected to receive additional funds as an invited Subsequent Phase II, Phase II Enhancement, or via the Commercialization Readiness Program (CRP). STTR Phase II awards may also be selected to receive additional funds as an invited Subsequent Phase II.

3. Phase III. In Phase III, the small business or research institute is expected to obtain funding from the private sector and/or non-SBIR/STTR government sources to develop products, production, services, R&D, or any combination thereof into a viable product or service for sale in military or private sector markets. Commercialization is the ultimate goal of the SBIR and STTR programs.

C. ARO FY16 SBIR and STTR Topics

The following SBIR and OSD Defense Health Program SBIR topics were published in the FY16 SBIR BAAs. The lead topic author (who serves as the topic PM) and corresponding Division are listed with each topic.

- *Enhanced Analysis for Pulsed Voltammetry Evaluation Tool / System For Improved Power Systems*; Dr. Robert Mantz, Chemical Sciences
- *High Quality Factor, Thin-Film, Electrically Tunable Varactors and Filters*; Dr. James Harvey, Electronics
- *Low-Loss Commercial Deposition Technology for Thick Ferrites and Ferrite/Insulator Films on Printed Circuit Boards*; Dr. James Harvey, Electronics
- *Optical Thin Film Technologies for High Energy Lasers*; Dr. Pani Varanasi, Materials Science
- *Artificial Vaccines Based on DNA Origami*; Dr. Stephanie McElhinny, Life Sciences

The following STTR topics were published in the FY16 STTR solicitations. The lead topic author and corresponding Division are listed following each topic title.

- *Compressive 3D Infrared Imaging*; Dr. Liyi Dai, Computing Sciences
- *Quantification Model and Systems for Assessing and Developing Resilient Wireless Communication Operation*; Dr. Cliff Wang, Computing Sciences
- *Field Drug Identification Kit*; Dr. Dawanne Poree, Chemical Sciences
- *Acoustically/Vibrationally Enhanced High Frequency Electromagnetic Detector for Buried Landmines*; Dr. James Harvey, Electronics
- *Green Diode Lasers (480-550 nm Spectral Regime)*; Dr. Michael Gerhold, Electronics
- *Situational Awareness System*; Dr. Edward Palazzolo, Network Sciences

D. ARO FY16 SBIR and STTR Phase II Contract Awards

The following SBIR topics were selected for Phase II contracts in FY16. The lead topic author/PM and corresponding Division are listed following each topic title.

- *Universal Software-Defined Receiver for Assured and Seamless Position, Navigation, and Timing (PNT)*; Dr. Joe Qiu, Electronics
- *Rapid Analysis of Suspicious Powders*; Dr. Bob Kokoska, Life Sciences
- *High Operating Temperature Long Wave HgCdTe Focal Plane Arrays*; Dr. William Clark, Electronics

- *Very High Dynamic Range RF Two Tone Measurement Instrument and Sensor*; Dr. James Harvey, Electronics
- *Oxygen Separation from Air to Provide Supplemental Oxygen for Injured Soldiers*; Dr. Robert Mantz, Chemical Sciences

The following STTR and CBD STTR topics were selected for Phase II contracts in FY16. The lead topic author/PM and corresponding Division are listed following each topic title.

- *Ultra-Coherent Semiconductor Laser Technology*; Dr. Michael Gerhold, Electronics
- *Powerful Source of Collimated Coherent Infrared Radiation with Pulse Duration Fewer than Ten Cycles*; Dr. James Harvey, Electronics
- *High-Performance Magnesium Alloys and Composites by Efficient Vapor Phase Processing*; Dr. David Stepp, Materials Science
- *Low Power Monolayer MoS2 Transistors for RF Application*; Dr. Pani Varanasi, Materials Science
- *Regulate Circadian Rhythm for Health and Performance*; Dr. Virginia Pasour, Mathematical Sciences
- *Cryogenic Low-Noise Amplifiers for Quantum Computing and Mixed-Signal Applications*; Dr. T.R. Govindan, Physics
- *Biologically-Derived Targeted Antimicrobials for Textile Applications*; Dr. Stephanie McElhinny, Life Sciences
- *Parallel Two-Electron Reduced Density Matrix Based Electronic Structure Software for Highly Correlated Molecules and Materials*; Dr. James Parker, Chemical Sciences
- *Advanced Computational Technologies for Multiphase Internal/External Coupled Ballistic Flows*; Dr. Joseph Myers, Mathematical Sciences
- *Intracavity Nonlinear Optical Generation of THz Radiation*; Dr. Michael Gerhold, Electronics
- *Stochastic Electromagnetic / Circuit Analysis*; Dr. James Harvey, Electronics
- *Terahertz Nano-Radio Platform with Integrated Antenna and Power Source*; Dr. Joe Qui, Electronics
- *Novel Lightweight Thermoacoustic Materials and Processes for Noise Cancellation of Military Ground Combat Vehicles (GCV)*; Dr. Pani Varanasi, Materials Science
- *Compressive 3D Infrared Imaging*; Dr. Liyi Dai, Computing Sciences
- *EMS Monitor & Broadcast Training Capacity Enhancement*; Dr. Robert Ulman, Network Sciences
- *Compact Integrated Ion Trap Quantum Systems*; Dr. T.R. Govindan, Physics
- *Lithium Ion / Super Capacitor Hybrid System*; Dr. Robert Mantz, Chemical Sciences
- *Advanced Fibers for High Efficiency Capture and Release of Human Cellular Material for Forensic DNA Analysis*; Dr. Stephanie McElhinny, Life Sciences
- *Robust Training System for Autonomous Detectors*; Dr. Micheline Strand, Life Sciences
- *Innovative Concept for Detection and ID of Biological Toxins*; Dr. Dawanne Poree, Chemical Sciences

E. ARO FY16 SBIR Sequential Phase II Contract Awards

The following SBIR and CBD SBIR topics were selected for Sequential Phase II contracts in FY16. The lead topic author/PM and corresponding Division are listed following each topic title.

- *Nanostructured Electrode Materials for Enhanced Biological Charge Transfer*; Dr. Stephanie McElhinny, Life Sciences
- *Inferring Social and Psychological Meaning in Social Media*; Dr. Joseph Myers, Mathematical Sciences
- *Ultra-Coherent Semiconductor Laser Technology*; Dr. Michael Gerhold, Electronics
- *Fabrication of High-Strength, Lightweight Metals for Armor and Structural Applications*; Dr. David Stepp, Materials Science
- *High Quality AlGaN Epitaxial Films with Reduced Surface Dislocation Density*; Dr. Pani Varanasi, Materials Science

- *Direct Ethanol Fuel Cell*; Dr. Robert Mantz, Chemical Sciences
- *Coherent Beam Combining of Mid-IR Lasers*; Dr. Michael Gerhold, Electronics
- *Rapid Detection System for Decontaminated Bacillus Thuringiensis Al Hakam Spore Strips*; Dr. Dawanne Poree, Chemical Sciences

F. ARO FY16 SBIR Phase II Enhancement Contract Awards

The following SBIR topics were selected for Phase II Enhancement contracts in FY16. The lead topic author/PM and corresponding Division are listed following each topic title.

- *UV-Enhanced Raman Sensors with High SNR and Spectral Selectivity*; Dr. Michael Gerhold, Electronics
- *Solid Acid Electrolyte Fuel Cell*; Dr. Robert Mantz, Chemical Sciences

G. ARO FY16 STTR Phase III Contract Awards

The following STTR and CBD STTR topics were awarded a Phase III contract in FY15 and FY16. The lead topic author/PM and corresponding Division are listed following each topic title. Phase III revenues can be obtained from Government or private customers, but cannot be SBIR/STTR funds.

- *Micro-Machined THz Probes for Electronic Analysis of Integrated Structures*; Dr. Joe Qiu, Electronics
- *Lithium Ion / Super Capacitor Hybrid System*; Dr. Robert Mantz, Chemical Sciences
- *Innovative Concept for Detection and ID of Biological Toxins*; Dr. Dawanne Poree, Chemical Sciences

H. Contract Evaluation and Funding

The Army receives Phase I and Phase II proposals in response to SBIR, STTR, CBD-SBIR and OSD-SBIR/STTR topics that are published during solicitation periods throughout each fiscal year. Proposals are evaluated against published evaluation criteria and selected for contract award. Contract awards are made pending completion of successful negotiations with the small businesses and availability of funds. A summary of funds managed for ARO-managed SBIR and STTR contracts is provided at the end of this chapter.

TABLE 2

Total Funding for ARO-managed SBIR and STTR contracts awarded in FY16. Total funding (FY16 and reallocated FY15 funds) for ARO-managed SBIR and STTR contracts, including Army, CBD, OSD, and other DoD funding sources. Phase III includes contracts deriving from, extending or completing ARO-managed Phase I or Phase II efforts, awarded at ARO and elsewhere within the DoD.

	SBIR Contracts	STTR Contracts
Phase I	$2,497K	$1,662K
Phase II	$2,593K	$12,937K
Phase II Enhancement	$1,000K	-
Sequential PH II	$5,367K	-
Phase III	$103K	$425K
TOTAL	$11,560K	$15,024K

IX. HISTORICALLY BLACK COLLEGES AND UNIVERSITIES AND MINORITY SERVING INSTITUTIONS (HBCU/MSI) PROGRAMS

Programs for HBCU/MSIs are a significant part of the ARO portfolio. Awards in FY16 totaled $22.3 million. These programs are discussed in the following subsections.

A. ARO (Core) HBCU/MSI Program

ARO began its HBCU/MSI program in 1980 with $0.5 million designed to encourage greater participation of HBCUs and MSIs in basic research. The initiative has continued and in recent years has been funded at about $1.2 million annually. These funds are made available to the ARO scientific divisions as co-funding opportunities to support HBCU/MSI research proposals submitted through the ARO Core Program BAA. There were 88 agreements with HBCU/MSI institutions receiving over $8.74 million in H57 funding through the ARO Core Program during FY16, including the 30 new starts. These figures represent total funding for HBCU/MSIs through the core program, both awards relying on matching funds and those not utilizing matching funds.

The new-start HBCU/MSI research grants are listed below, with the project title followed by the PI, performing organization, ARO PM, and corresponding scientific division.

- *Tasks and Transitions: An Investigation of Transactive Memory Systems in Teams Performing Multi-Task Activities*, Professor Kyle Lewis, University of California - Santa Barbara; Dr. Edward Palazzolo, Network Sciences

- *Dissecting Social Dynamics and Malware Attributions for Mitigating Network-centric Attacks*, Professor Gail-Joon Ahn, Arizona State University; Dr. Cliff Wang, Computing Sciences

- *Spatial-temporal memory effects in nanoelectronic neuromorphic networks*, Professor Dmitri Strukov, University of California - Santa Barbara; Dr. Joe Qiu, Electronics

- *Integrated Cognitive Mobile and Social Networking*, Professor Junshan Zhang, University of Arizona; Dr. Robert Ulman, Network Sciences

- *Towards Optimal Teams in Composite Networks*, Professor Hanghang Tong, Arizona State University; Dr. Edward Palazzolo, Network Sciences Division

- *Epitaxial Cd3As2 for RF Device Applications*, Professor Robert York, University of California - Santa Barbara; Dr. James Harvey, Electronics

- *Extending the Mechanisms of Protein Function to Non-Cellular Environments*, Professor Sumita Pennathur, University of California – Santa Barbara; Dr. Stephanie McElhinny, Life Sciences

- *Correlative study of defects in semiconductors*, Professor Yong Zhang, University of North Carolina – Charlotte; Dr. Michael Gerhold, Electronics

- *The II-IV Nitrides materials system as a novel design space for quantum materials*, Professor Christian Van de Walle; University of California – Santa Barbara; Dr. Pani Varanasi, Materials Science

- *Trustworthy Human Centric Social Networking: Challenges and Research*, Professor Yanchao Zhange, Arizona State University; Dr. Cliff Wang, Computing Sciences

- *Microscale Ocean Biophysics*, Professor Shilpa Khatri, University of California - Merced; Dr. Virginia Pasour, Mathematical Sciences

- *24th Current Trends in Computational Chemistry*, Professor Jerzy Leszczynski, Jackson State University; Dr. James Parker, Chemical Sciences

- *Individual Differences in Handedness Effects on Categorical versus Coordinate Spatial Processing*, Professor Ruth Propper, Montclair State University; Dr. Frederick Gregory, Life Sciences

- *Theoretical Foundations, Modeling, and Exploration for Power Obfuscation in Secure Embedded Systems*, Professor Roman Lysecky, University of Arizona; Dr. Cliff Wang, Computing Sciences

- *Octree Methods for Multiscale Discretization,* Professor Frederic Gibou, University of California – Santa Barbara; Dr. Joseph Myers, Mathematical Sciences

- *A New Approach to the Combustion Chemistry of Low Cetane Number Jet Fuels*, Professor Kenneth Brezinsky, University of Illinois – Chicago; Dr. Ralph Anthenien, Mechanical Sciences Division

- *Ultrafast Light Emitters Using Photonic Hypercrystals and Two Dimensional Semiconductors*, Professor Vinod Menon, City University of New York (CUNY); Dr. Michael Gerhold, Electronics

- *Vertical Transport in lnAs/InAsSb Superlattices, Professor Sanjay Krishna*, University of New Mexico-Albuquerque; Dr. Michael Gerhold, Electronics

- *Predicting and managing migration: insights from age-structured, game-theoretic, and network models*, Professor Maria-Rita D'Orsogna, California State University - Northridge; Dr. Purush Iyer, Network Sciences

- *Towards Synthetic Nonabelions in Graphene Heterostructures,* Professor Andrea Young, University of California - Santa Barbara; Dr. Marc Ulrich, Physics

- *Proof of Concept for Efficient Application of Quantum-Chemical Techniques to Model Environmental Mercury Depletion Reactions Through Transition State Theory*, Professor Jerzy Leszczynski, Jackson State University; Dr. James Parker, Chemical Sciences

- *Gathering and Processing Sensor Data with Unmanned Relay Vehicles using Line-of-Sight Communication*, Professor Leonardo Bobadilla, Florida International University; Dr. Liyi Dai, Computing Sciences

- *The Impact of Landscape Characteristics on Urban Surface Energy Balance,* Professor Zhihua Wang, Arizona State University; Dr. Julia Barzyk, Materials Sciences

- *The Chaotic Quantum Oscillator*, Professor Bjorn Birnir, University of California - Santa Barbara; Dr. James Harvey, Electronics

- *Mechanoresponsive Polymer-Matric Composites*, Professor Matthew Green, Arizona State University; Dr. Dawanne Poree, Chemical Sciences

- *Scientific Exploration of Cyber-Driven Dynamic, Distributed Big Data Forensics Systems*, Professor Sundararaj Iyengar, Florida International University; Dr. Cliff Wang, Computing Sciences

- *Tailoring Vibrational Modes and Interactions in Resonators and Waveguides: Multiscale Model of Phonon and Phonon Interactions - Transition from MEMS to NEMS*, Professor Michael Stroscio, University of Illinois – Chicago; Dr. James Harvey, Electronics

- *Canonical Tensors Applied to Ab Initio Electronic Structure: Linear Scaling for Metallic Systems,* Professor Christopher Tymczak, Texas Southern University; Dr. James Parker, Chemical Sciences

- *Epitaxial superconductor-semiconductor two-dimensional systems: a new platform for quan-tum computation*, Professor Javad Shabani, City College of New York (CUNY); Dr. T.R. Govindan, Physics

- *Nanostructured High Entropy Alloys,* Professor Enrique Lavernia, University of California - Irvine; Dr. Michael Bakas, Materials Science

The HBCU/MSI institutions funded under the ARO Core program were also afforded the opportunity to submit add-on proposals to fund high school or undergraduate student research apprenticeships through HSAP/URAP. A total of 17 HBCU/MSIs were funded under HSAP/URAP in FY16, totaling approximately $154K, (50/50 mix of PM and Army Education Outreach Program funding). Additional information regarding HSAP/URAP can be found in Section XI: *Youth Science Activities*.

B. Partnership in Research Transition (PIRT) Program

The PIRT Program was established as the second phase of what was previously known as the Battlefield Capability Enhancement Centers of Excellence (BCE). The program's objective is to enhance the programs and capabilities of a select number of high-interest scientific and engineering disciplines through Army-relevant, topic-focused, near-transition-ready innovative research. Furthering ARL's policy of advocating and supporting research at HBCUs, and consistent with the stated mission of the White House Initiative on HBCUs, a secondary objective of PIRT is "to strengthen the capacity of HBCUs to provide excellence in education" and to conduct

research critical to DoD national security functions. In FY16, $1.7 million was added to Cooperative Agreements supporting research and student internships at these PIRT Centers:

- *Center of Advanced Algorithms*
  Delaware State University, Dover, DE
  Co-Cooperative Agreement Manager (Co-CAM): Dr. James Harvey, Electronics

- *Bayesian Imaging and Advanced Signal Processing for Landmine and IED Detection Using GPR*
  Howard University, Washington, DC
  Co-CAM: Dr. James Harvey, Electronics

- *Extracting Social Meaning From Linguistic Structures in African Languages*
  Howard University, Washington, DC
  Co-CAM: Dr. Joseph Myers, Mathematical Sciences

- *Lower Atmospheric Research Using Lidar Remote Sensing*
  Hampton University, Hampton, VA
  Co-CAM: Dr. James Parker, Chemical Sciences

- *Multi-Scale Modeling Techniques and Analysis for Cementitious Materials Under Dynamic Loading*
  North Carolina A&T State University, Greensboro, NC
  Co-CAM: Dr. Joseph Myers, Mathematical Sciences

C. DoD Research and Educational Program (REP) for HBCU/MSI

ARO has administered programs on behalf of ASD(R&E) since 1992. REP aims to enhance research capabilities of HBCUs and MSIs and to strengthen their education programs in science, technology, engineering, and mathematics (STEM) disciplines that are relevant to the defense mission.

Under this program, qualifying institutions were able to submit proposals to compete for basic research grants. In FY16, BAA W911NF-16-R-0024 was issued for the DoD REP for HBCUs/MSIs.   One hundred sixty-two (162) proposals were determined to be eligible under the solicitation. In FY16, 76 grants totaling $29.2M were made, 29 to HBCUs, 46 to MSIs, and 1 to a TCU under the DoD REP solicitation.

D. Other HBCU/MSI Activities

ARO completed administration of the John H. Hopps Scholars Program at Morehouse College (FY08-FY16), which continued to serve nine scholars during FY16. ARO also provided support to AMC and RDECOM to develop an Army Strategic Plan to address Section 233 of the National Defense Authorization Act (NDAA).

X. NATIONAL DEFENSE SCIENCE AND ENGINEERING GRADUATE (NDSEG) FELLOWSHIP PROGRAM

The NDSEG Fellowship Program is a tri-service program administered by the Air Force Office of Scientific Research (AFOSR), designed to increase the number of US citizens trained in disciplines of science and engineering important to defense goals. ARO supports the NDSEG Fellowship Program along with the Office of Naval Research (ONR) and AFOSR. NDSEG is a highly competitive fellowship awarded to U.S. citizens who have demonstrated a special aptitude for advanced training in science and engineering, and who intend to pursue a doctoral degree in one of fifteen scientific disciplines of interest to the military. NDSEG Fellowships last for three years, and Fellows are provided full tuition and fees at any accredited university of choice, a monthly stipend very competitive with other top-tier fellowships, and up to $1K/year in medical insurance.

With approximately $5 million available to the Army in FY16, ARO selected 60 NDSEG Fellows from thirteen categories relevant to Army fundamental research priorities. These awardees began their fellowships in the fall of 2016. Each of ARO's divisions reviewed the applications assigned to NDSEG topic categories within their particular areas of expertise, and selected fellows whose doctoral research topics most closely align with the

Army's missions and research needs. The number of Fellows chosen from each discipline was based roughly on the percentage of applicants who submitted topics in that category. The number of fellows chosen from each scientific discipline for the FY16 NDSEG program is shown in TABLE 2.

TABLE 2

FY16 NDSEG fellows by discipline. The table displays the number of NDSEG Fellows chosen in FY16, according to topic categories relevant to the designated Army research priorities.

Scientific Discipline	NDSEG Fellows Selected in FY16
Aeronautical and Astronautical Engineering	3
Biosciences	10
Chemical Engineering	4
Chemistry	7
Civil Engineering	2
Cognitive, Neural, and Behavioral Sciences	5
Computer and Computational Sciences	4
Electrical Engineering	4
Geosciences	2
Materials Science and Engineering	7
Mathematics	3
Mechanical Engineering	5
Physics	4
TOTAL	**60**

XI. YOUTH SCIENCE ACTIVITIES

All the programs managed by the Army Educational Outreach Program (AEOP) STEM Outreach Office at RDECOM Headquarters share one purpose: to increase the number of future adults with careers in science, technology, engineering, and mathematics. These programs accomplish this through a variety of mechanisms, including: providing a work/study laboratory experience, sponsoring hands-on science workshops during the summer, showcasing talented young high school scientists at symposia, and supporting student science fairs nationwide. Of these many programs, ARO continued to administer the High School and Undergraduate Research Apprenticeship Programs in FY16.

During the summer of FY16, 117 students served as interns and worked in university laboratories with mentors though the High School Apprenticeship Program (HSAP) and the Undergraduate Research Apprentice Program (URAP). This was a significant increase from the number of participants in FY15. These programs are described further in the following subsections.

A. Undergraduate Research Apprenticeship Program (URAP)

URAP funds the STEM apprenticeship of promising undergraduates to work in university-structured research environments under the direction of ARO-sponsored PIs serving as mentors. In FY16, URAP awards provided

52 students with research experiences at 39 different universities within 22 different states. Fourteen of the universities were HBCU/MSIs and ARO invested approximately $203K in the FY16 URAP effort, a mix of ARO core funding and AEOP matching funds.

B. High School Apprenticeship Program (HSAP)

HSAP funds the STEM apprenticeship of promising high school juniors and seniors to work in university-structured research environments under the direction of ARO-sponsored PIs serving as mentors. In FY16, HSAP awards provided 65 students with research experiences at 35 different universities within 18 different states. Sixteen of the universities were HBCU/MSIs. ARO invested approximately $236K in the FY16 HSAP effort, including ARO core funding and AEOP matching funds.

C. Thurgood Marshall College Fund Pilot Initiative

The Vivian Burey Marshall Academy (VBMA), named in honor of Justice Thurgood Marshall's first wife, is a two-tiered, pilot initiative grant awarded to the Thurgood Marshall College Fund in late FY16. This is a four-year research grant award up to $5.7 million funded by ASA (ALT) through ARL's Broad Agency Announcement and consistent with the goals of the AEOP. The pilot initiative will develop in young students, grades 6-10, STEM literacy and the basic underlying skills necessary for STEM management.

The pilot effort will be evaluated throughout the 4-year implementation to assess impact and feasibility of program adoption. ASA (ALT) has requested Army science and technology (S&T) organizations support VBMA sites for the initial year: RDECOM with Baltimore, MD, and ERDC with Vicksburg, MS.

D. Local Outreach

The Youth Sciences division of ARO participated in the following local outreach efforts in FY16.

- North Carolina Science and Engineering Fair: ARO PMs volunteered to judge posters for a special category that presents awards to high school juniors and seniors based upon the overall quality and Army relevance of their projects.
- Regional JSHS: ARO attended and judged high school student posters for the regional competition. Top winners advance to the national JSHS competition.
- JSHS National Symposium: scientists from ARO and sponsored PIs attended and judged student posters as well as oral presentations of students that have previously won regional competitions. Winners are awarded various scholarships ranging from $4,000 to $12,000.
- Site visits to local universities that host HSAP/URAP participants: the HSAP/URAP Program Coordinator visited host sites within North Carolina to measure program efficacy. An ARO PM accompanied the Program Coordinator on three of the visits.
- Arts n' STEM Expo: ARO joined US2020 RTP, a nonprofit organization that facilitates Science, Technology, Engineering and Mathematics outreach and mentoring opportunities for underrepresented minorities, during their "Arts n' STEM" expo. Program Managers from ARO in the fields of chemistry, physics, mathematics and environmental, social and life sciences volunteered as speed mentors to an estimated 350 students ranging from grades 5 to 12 at the Frontier building in Research Triangle Park, North Carolina. The Youth Science Program Coordinator also staffed a display promoting Army Educational Outreach Programs, including HSAP and URAP, at the event.

XII. SCIENTIFIC SERVICES PROGRAM (SSP)

ARO established the SSP in 1957. This program provides a rapid means for the Army, DoD, OSD, and other federal government agencies to acquire the scientific and technical analysis services of scientists, engineers, and analysts from small and large businesses, colleges and universities, academicians working outside their institutions, and self-employed persons not affiliated with a business or university. Annual assistance is provided through the procurement of short-term, engineering and scientific technical services in response to user-agency requests and funding. Through the SSP, these individuals provide government sponsors with scientific and technical results and solutions to problems related to R&D by conducting well-defined studies, analyses, evaluations, interpretations, and assessments in any S&T area of interest to the government.

SSP services are administered and managed for ARO through the Battelle Eastern Science and Technology (BEST) Center located in Aberdeen, Maryland on behalf of Battelle Memorial Institute (BMI), headquartered in Columbus, Ohio. Battelle's responsibilities include the selection of qualified individuals, universities, businesses, and/or faculty to perform all tasks requested by ARO, and for the financial, contractual, security, administration, and technical performance of all work conducted under the program.

SSP awards tasks in a wide variety of technical areas, including mechanical engineering, computer sciences, life sciences, chemistry, material sciences, and military personnel recruitment/retention. In FY16, 35 new SSP tasks were awarded with 106 modifications to the scope and/or funding of ongoing tasks. A summary of the agencies served under this program and the corresponding number of FY16 new SSP tasks is provided in TABLE 3.

TABLE 3

FY16 new SSP tasks and sponsoring agencies. In FY16, 35 new SSP tasks were awarded in addition to 106 modifications of the scope and/or funding of ongoing tasks on two SSP contracts.

Sponsoring Organization	SSP Tasks
Army Research, Development and Engineering Command (RDECOM)	
Army Research Laboratory (ARL)	3
Edgewood Chemical, Biological Center (ECBC)	6
Army Missile RDEC (AMRDEC)	3
Natick Soldier RDEC (NSRDEC)	4
TOTAL: RDECOM	**16**
Other U.S. Army	
US Military Academy (USMA)	1
Army Materiel Systems Analysis Activity (AMSAA)	1
Program Executive Office Ground Combat Systems	1
US Army Corps of Engineers (USACE)	3
US Army Training & Doctrine Command (TRADOC)	1
US Army Medical Command (MEDCOM)	7
TOTAL: Other U.S. Army	**14**
Other DoD	
US Navy	3
DoD (Other)	2
TOTAL: Other DoD	**5**
TOTAL FY16 SSP Tasks	**35**

XIII. SUMMARY OF PROGRAM FUNDING AND ACTIONS

A. FY16 Research Proposal Actions

ARO PMs receive white papers throughout the year and discuss these topic ideas with the potential investigator to identify any ways the proposed research could better align with program vision and Army needs. PMs then encourage a subset of white papers to be submitted as full proposals; however, any eligible investigator can submit a full proposal, regardless of PM recommendations. On average, one-fifth of the white papers received by ARO PMs are ultimately submitted as formal, full proposals.

The actions for FY16 extramural basic research full proposal submissions, sorted by ARO Division, are summarized in TABLE 4.

TABLE 4

FY16 ARO Research Proposal Actions. The status of research proposals received by ARO within FY16 (*i.e.*, 1 Oct 2015 through 30 Sep 2016) is listed for each scientific division, based on proposal actions reported through 14 July 2017. The table reports actions for extramural proposals in the basic research categories: SI, STIR, YIP, HBCU/MSI, REP, MRI, MURI, and DURIP.

	Received	Accepted	Declined	Pending	Withdrawn
Chemical Sciences	129	50	44	35	0
Computing Sciences	62	31	11	20	0
Electronics	109	39	45	25	0
Life Sciences	95	42	34	19	0
Materials Science	91	45	30	13	3
Mathematical Sciences	44	21	18	5	0
Mechanical Sciences	72	27	28	17	0
Network Sciences	68	44	14	10	0
Physics	80	33	33	14	0
TOTAL	**750**	**332**	**257**	**158**	**3**

B. Summary of ARO Core Program Budget

The ARO FY16 Core (BH57) Research Program budget is shown in TABLE 5, below.

TABLE 5

ARO Core (BH57) Program funding. The ARO Core Program FY16 Budget is listed according to each scientific discipline (Division) or special program; data sources: ARO Director's Budget (for scientific disciplines) and Status of Funds Report 28 Feb 2017 (for special programs).

ARO Core (BH57) Program Type	Division or Program Title	FY16 Allotment
Scientific Disciplines	Chemical Sciences[1]	$8,001,883
	Computing Sciences	$5,261,008
	Electronics	$6,978,782
	Life Sciences	$7,699,718
	Materials Science[1]	$8,648,374
	Mathematical Sciences	$5,929,016
	Mechanical Sciences	$7,422,453
	Network Sciences	$7,065,732
	Physics	$7,048,878
	SUBTOTAL: Core Program Funding by Scientific Discipline	**$66,055,438**
Special Programs	Senior Scientist Research Programs	$877,456
	International Offices	$1,230,997
	National Research Council (NRC) Associates Program	$462,656
	HBCU/MSI Program[2,3]	$786,293
	HSAP/URAP	$181,268
	In-House Operations	$16,919,892
	SUBTOTAL: Core Program Funding to Special Programs	**$20,458,562**
TOTAL	**ARO Core (BH57) Program**	**$84,514,406**

[1] Includes funding for some projects that began under the former Environmental Sciences Division, now temporarily managed within these other Divisions.

[2] HBCU/MSI Core Program funds are allocated at the Directorate level, and are matched with Division funds, resulting in total FY16 HBCU/MSI Core Program funding of $1.5M.

[3] Does not include the additional funds provided from OSD for the HBCU/MSI Program (see TABLE 8).

C. Summary of Other Programs Managed or Co-managed by ARO

The FY16 allotments and funding sources for other ARO managed or co-managed programs (*i.e*, not part of the ARO Core Program), are shown in TABLES 6-8.

TABLE 6

FY16 allotments for other Army-funded programs. These programs, combined with the ARO Core (BH57) Program elements shown in TABLE 5, represent all of the Army-funded programs managed through ARO. Data source: ARO Director's Budget and 30 Sep 2016 Status of Funds Report (for FY15 funds received in or reallocated for FY16).

Other Army-funded Program	FY16 Allotment
Multidisciplinary University Research Initiative	$44,845,496
Presidential Early Career Award for Scientists and Engineers	$2,897,748
Defense University Research Instrumentation Program	$12,118,203
University Research Initiative Support	$4,453,553
MINERVA Program (Project V72)[1]	$2,910,000
Army Center of Excellence (Project H59)	$509,000
HBCU/MSI – PIRT Centers (Project H04)	$1,812,000
Army Institute for Collaborative Biotechnologies (ICB; Project H05)	$6,228,000
Army Institute for Soldier Nanotechnologies (AISN; Project J12)	$5,339,000
Army Institute for Creative Technologies (AICT; Project J08)	$5,839,000
Board of Army Science and Technology (BAST; Project C18)	$1,399,000
Small Business Innovation Research (SBIR; Project M40)[1,2]	$7,848,342
Small Business Technology Transfer (STTR; Project 861)[1]	$12,875,062
SBIR/STTR Services / Contract Support (Project 720)	$746,079
Basic Research Initiatives – Congressional (T14)	$15,000,000

TOTAL: Other Army-funded Programs $124,820,483

[1] Does not include additional funds provided by OSD (see TABLE 8).
[2] Includes $3,612,941 of FY15 funds received in or reallocated for FY16

TABLE 7

FY16 allotment for externally-funded programs. FY16 funds received from sources other than Army or OSD are indicated below. The Other Agencies category totals the funds from a range of sources, including the Joint IED Defeat Organization (JIEDDO), the Joint Project Manager, Nuclear, Biological, and Chemical (JPMNBC), and other government agencies. Data source: 31 Jan 2017 Status of Funds Report and 30 Sep 2016 Status of Funds Report (for FY15 funds received in or reallocated for FY16).

External Program	FY16 Allotment
Scientific Services Program (SSP)[1]	$9,182,239
Defense Advanced Research Projects Agency (DARPA)[2]	$170,217,670
Air Force Research Laboratory (AFRL)	$4,059,911
Other Agencies (*e.g.*, JIEDDO and JPMNBC)	$53,398,518
Other DoD	$51,436,870
TOTAL: External Programs	**$288,295,208**

[1] Includes $145,477 of FY15 funds received in or reallocated for FY16
[2] Includes $16,718,543 of FY15 funds received in or reallocated for FY16

TABLE 8

OSD direct-funded programs. These funds were allocated directly from OSD to the indicated program. Data source: 31 Jan 2017 Status of Funds Report.

OSD Direct-funded Programs	FY16 Allotment
SBIR/STTR (Project 8Z5)[1,2]	$1,745,678
Basic Research Initiatives - Congressional	$441,000
HBCU/MSI and Research and Educational Program (REP)[3,4]	$34,138,000
Minerva[5]	$13,122,052
TOTAL: OSD Direct Funding	**$49,446,730**

[1] Does not include additional Army funds provided for SBIR/STTR (see TABLE 6).
[2] This allotment was FY15 funds received in or reallocated for FY16
[3] This amount does not include the additional Army Core Program funds provided for the HBCU/MSI Program (see TABLE 5).
[4] Includes $2,292,000 of FY15 funds received in or reallocated for FY16
[5] Includes $6,188,710 of FY15 funds received in or reallocated for FY16

D. Grand Total FY16 Allotment for ARO Managed or Co-managed Programs

TABLE 9

Summary of FY16 allotment for all ARO managed or co-managed programs. This table lists the subtotals from TABLES 6-9 and the grand total FY16 allotment for all ARO managed or co-managed programs, including any FY15 funds received in or allocated for FY16. Refer to TABLES 6-9 for data source information.

Program Category	FY16 Allotment
Core (BH57) Programs	$84,514,406
Other Army-funded Programs	$124,820,483
External Program Funds	$288,295,208
OSD Direct-funded Programs	$49,446,730
GRAND TOTAL: (all sources)	**$547,076,827**

CHAPTER 3: CHEMICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2016* is to provide information on the programs and basic research supported by ARO in FY16, and ARO's mission to create basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Chemical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and transitions facilitated by this Division in FY16.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Chemical Sciences Division supports research to identify and control the fundamental properties, principles, and processes governing molecules and their interactions in materials and chemical systems that will ultimately enable critical new Army capabilities. More specifically, the Division promotes basic research to uncover the relationships between molecular architecture and material properties, to understand the fundamental processes of electrochemical reactions, to develop methods for accurately predicting the pathways, intermediates, and energy transfer of reactions, and to discover and characterize the many chemical processes that occur at surfaces and interfaces. The results of these efforts will stimulate future studies and help keep the U.S. at the forefront of chemical sciences research. In addition, these efforts are expected to lead to new approaches for synthesizing and analyzing molecules and materials that will open the door to future studies that are not feasible with current knowledge.

2. Potential Applications. Research managed by the Chemical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, results from the Chemical Sciences Program may lead to materials with new or enhanced properties to protect the Soldier from ballistic, chemical, and biological threats. The development of new computational methods may allow the structure and properties of notional (*i.e.*, theoretical) molecules to be calculated before they are created, providing a significant cost savings to the Army. In addition, chemical sciences research may ultimately improve Soldier mobility and effectiveness through the development of light-weight and small power sources, renewable fuel sources, and new energetic materials with improved methods for ignition, detonation, and control.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Chemical Sciences Division coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AFOSR). In addition, the Division coordinates with other ARO Divisions to co-fund research, identify multidisciplinary research topics, and to evaluate the merit of research concepts. For example, interactions with the ARO Life Sciences Division include developing research programs to investigate materials for use in chemical and biological defense and to understand how biological systems can interface with or expand the capabilities of abiotic systems. The Chemical Sciences Division also coordinates its research portfolio with the Materials Science Division to pursue the design and characterization of novel materials through new synthesis and processing methods, the evaluation of bulk mechanical properties, and molecular-level studies of materials and material properties. The Division also complements research in the Physics and Electronics Divisions to investigate the dynamics of chemical reactions and how chemical structure influences electrical, magnetic, and optical properties. The creation of new computational methods and models to better understand molecular structures and chemical reactions is also an area of shared interest between the Chemical Sciences and Mathematical Sciences Divisions.

In addition, the Division's research portfolio will reveal previously unexplored avenues for new Army capabilities while also providing results to support (i) the Materials Research Campaign's goals to create multifunctional, responsive materials, and to discover and exploit materials for more efficient power generation and energy storage, (ii) the Sciences-for-Maneuver Campaign's goals to identify and exploit innovations in energy sources, storage, and conversion, to discover novel materials to enable durable, damage tolerant structural systems, to discover materials to enable damage-tolerant structural systems, and to engineer and exploit chemical systems with biological-like functions for advanced protective equipment, and (iii) the Sciences for Lethality-and-Protection Campaign's goal to develop new energetic materials and predictive models of their behavior.

B. Program Areas

The Chemical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the identification, evaluation and monitoring of research projects. In FY16, the Division managed research within these five Program Areas: (i) Polymer Chemistry, (ii) Molecular Structure and Dynamics, (iii) Electrochemistry, and (iv) Reactive Chemical Systems. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Polymer Chemistry. The goal of this Program is to understand the molecular-level link between polymer microstructure, architecture, functionality, and the ensuing macroscopic properties. Research in this Program may ultimately enable the design and synthesis of functional polymeric materials that give the Soldier new and improved protective and sensing capabilities as well as capabilities not yet imagined. This Program is divided into two research thrusts: (i) Precision Polymeric Materials and (ii) Complex Polymer Systems. The Precision Polymeric Materials thrust supports research aimed at developing new approaches for synthesizing polymers with precisely-defined molecular weight, microstructure (monomer sequence and tacticity), architecture, and functional group location; exploring how changes in molecular structure and composition impact macroscopic properties; and on developing polymers that exhibit programmed molecular responses to external stimuli. Of particular interest is research related to sequence-defined polymers, self-immolative polymers, and polymer mechanochemistry. The Complex Polymer Systems thrust focuses on controlling polymer assembly to enable complex structures with diverse functions and new properties. Of interest to this thrust are research efforts that explore how molecular structure influences polymer assembly into more complex, hierarchical structures as well as influence interactions with other materials (*i.e.* inorganic or biological materials) to render functional hybrid assemblies. Research efforts that explore assembly/incorporation of multiple responsive groups into a single polymeric materials system to engender complex responsive behavior are also of interest.

The research supported by this Program Area may lead to long-term applications for the Army such as light-weight, flexible body armor, materials for clothing that are breathable but also provide protection from toxins, and fuel cell membranes to harness renewable energy. In addition, the efforts in this program may ultimately lead to new, dynamic materials such as photohealable polymers that can be used as a repairable coating and mechanically- or thermally-responsive polymers and composites that can convert external forces to targeted internal chemical reactions (*i.e.*, to convert external force to internal self-sensing and self-repair).

2. Molecular Structure and Dynamics. The goal of this Program Area is to understand state-selected dynamics of chemical reactions of molecules in gas and condensed phases across a wide variety of conditions, and to develop theories capable of accurately describing and predicting these phenomena. In the long term, these studies may serve as the basis for the design of future propellants, explosives, and sensors. This Program Area is divided into two Thrusts: (i) Molecular Dynamics and (ii) Quantitative Theoretical Methods. The Molecular Dynamics Thrust broadly supports research on the study of energy transfer mechanisms in molecular systems. The Quantitative Theoretical Methods Thrust supports research to develop and validate theories for quantitatively describing and predicting the properties of chemical reactions and molecular phenomena.

The research supported by this Program Area will likely enable many future applications such as more efficient and clean combustion technology, the capability to accurately predict the properties of large, complex chemical systems, and the development of novel molecules for use in energy storage applications.

3. Electrochemistry. The goal of this Program Area is to understand the underlying science that controls reactant activation and electron transfer. These studies may provide the foundation for developing advanced power generation and storage technology. This Program Area is divided into two research Thrusts: (i) Reduction-oxidation (Redox) Chemistry & Electrocatalysis, and (ii) Transport of Electroactive Species. The Redox Chemistry and Electrocatalysis thrust supports research to discover spectroscopic and electrochemical techniques for probing surfaces and selected species on those surfaces, while the Transport of Electroactive Species thrust identifies and supports research to uncover the mechanisms of transport through polymers and electrolytes, to design tailorable electrolytes based on new polymers and ionic liquids, and explores new methodologies and computational approaches to study the selective transport of species in charged environments.

Research in this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications include the discovery and use of new mechanisms for the storage and release of ions that are potentially useful in future power sources, including new battery or bio-fuel concepts. In addition, studies of electroactive species may enable the development of multifunctional materials that simultaneously have ionic conductivity, mechanical strength, and suitable electronic conductivity over a considerable temperature range, while exposed to aggressive chemical environments.

4. Reactive Chemical Systems. The goals of this Program Area are to obtain a molecular level understanding of interfacial activity and of dynamic nanostructured and self-assembled chemical systems. High-risk basic research in this program is expected to lead to the design and synthesis of new chemical systems that will provide unprecedented hazardous materials management capabilities and soldier survivability. This Program Area is divided into two research Thrusts: (i) Interfacial Activity and (ii) Synthetic Molecular Systems. Within these Thrusts, high-risk, high-payoff research efforts are identified and supported to pursue the program's long-term goals. The Interfacial Activity Thrust supports research on understanding the kinetics and mechanisms of reactions occurring at surfaces and interfaces and the development of new methods to achieve precise control over the structure and function of chemical and biological molecules on surfaces. Specific areas of interest include adsorption, desorption, and the catalytic processes occurring at surfaces and interfaces and the interface between nanostructures and biomolecules to generate advanced materials. Research in the Synthetic Molecular Systems Thrust is exploring novel methods for incorporation of multi-functionality, stimuli-responsive, and dynamic behavior into chemical systems. Specific areas of interest include the stabilization of nanostructured and self-assembled systems, incorporation of enhanced catalytic activity into chemical systems, and the design and synthesis of chemical systems that sense and respond to specific external stimuli.

This Program Area supports research that will likely lead to many long-term applications for the Army and the private sector. Potential long-term applications include novel chemical sensing capabilities, selective membranes, multi-functional surfaces for self-repair and self-healing, and new approaches to hazardous waste management. Research in these areas may also lead to multi-functional and stimuli-responsive systems for "smart" materials that can sense and autonomously respond in unprecedented ways for soldier protection.

C. Research Investment

The total funds managed by the ARO Chemical Sciences Division for FY16 were $53.3 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY16 ARO Core (BH57) program funding allotment for this Division was $8.0 million and $1.3 million of Congressional funds (T14). The DoD Multidisciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $11.5 million to projects managed by the Division. The Division also managed $16.8 million of Defense Advanced Research Projects Agency (DARPA) programs, and $2.5 million provided by other government agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $4.5 million for contracts. The Army's Institute for Soldier Nanotechnologies received $7.7 million. Finally, $1.2 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which included $0.2 million of the Division's total ARO Core (BH57) funds, in addition to funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY16 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY16 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY16, the Division awarded 20 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Rodney Bartlett, University of Florida - Gainesville; *Molecular Structure and Dynamics: Potential Energy Surfaces for Attosecond Spectroscopic Simulations*
- Professor Seth Cohen, University of California - San Diego; *Mixed-Matrix Membranes and Fibers*
- Professor David Flaherty, University of Illinois - Urbana-Champaign; *Mechanisms for Catalytically Abating Organosulfur Compounds with H_2O_2 Formed In Situ*
- Professor Samuel Gellman, University of Wisconsin - Madison; *Effects of Nanoscale Chemical Heterogeneity on Hydrophobic Interactions and Molecular Assembly at Surfaces*
- Professor Thomas Glover, University of South Alabama; *Development of Biocidal Fabrics Using the Reactive Dye Method*
- Professor Ayman Karim, Virginia Polytechnic Institute and State University; *Supported Single Atom Catalysts for Low Temperature Oxidation*
- Professor Anna Krylov, University of Southern California; *Metastable Autoionizing States of Molecules and Radicals in Highly Energetic Environment*
- Professor Benjamin Lear, Pennsylvania State University; *On Demand, Rapid, and Tunable Curing of Thermoset Polymers using the Photothermal Effect of Nanoparticles*
- Professor David Mazziotti, University of Chicago; *Effect of Strong Electron Correlation in the Description and Design of Efficient Energy-Transfer Mechanisms*
- Professor Kevin Noonan, Carnegie Mellon University; *Controlling Sequence in Precise Semiconducting Polymers*
- Professor Stephen Paddison, University of Tennessee - Knoxville; *Elucidating Correlation of Morphology with Charge Transport in Polymerized Ionic Liquids*
- Professor Herschel Rabitz, Princeton University; *Optimal Dynamic Control of Multiple Quantum Systems for Multiplexed Bio-network Analysis and Optogenetics*

- Professor James Radich, Auburn University; *Photoelectrochemical Hydrogen Production from Urea*

- Professor Robson Storey, University of Southern Mississippi; *Structure, Morphology, Property Relationships in Polyisobutylene-Based Triphasic Block Copolymers Containing Hydrophilic/Functional Block Elements*

- Ms. Beth Anne Stuebe, The Electrochemical Society; *Digitization Project To Make A Large Volume Of Content Hosted Online And To Digitize The Molten Salts Compendium*

- Professor Rein Ulijn, CUNY; *Transient Nanopatterns by Biocatalytic Self-Assembly*

- Professor Krista Walton, Georgia Tech Research Corporation; *Advanced Processing of Multifunctional Materials for Adsorptive Removal and Sensing of Chemical Warfare Agents*

- Professor Yan Xia, Stanford University; *Catalytic Synthesis of Shape-Persistent Ladder Polymers and Control of Their Intrinsic Microporosity*

- Professor Ting Xu, University of California - Berkeley; *Rational Design of Random Copolymers to Incorporate Proteins into Synthetic Materials*

- Professor Richard Zare, Stanford University; *Preparation of highly vibrationally excited H_2 molecules by Stark induced adiabatic Raman passage*

2. Short Term Innovative Research (STIR) Program. In FY16, the Division awarded 3 new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Kuppuswamy Arumugam, Wright State University; *Electrochemically Controlling the Ring Size and Molecular Topology of Cyclic Polyesters*

- Professor Matthew Green, Arizona State University; *Mechanoresponsive Polymer-Matrix Composites*

- Professor Wei You, University of North Carolina - Chapel Hill; *Controlled Chain-Growth Polymerization of Donor-Acceptor Conjugated Monomers*

3. Young Investigator Program (YIP). In FY16, the Division awarded one new YIP project to drive fundamental research in areas relevant to the current and future Army. The following PI and corresponding organization was awarded the new-start YIP project.

- Professor Adam Hauser, University of Alabama - Tuscaloosa; *Interdigitated Capacitor Devices for Airborne Chemical Sensing of Explosive Materials*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY16 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *15th Polymer Electrolyte Fuel Cell Symposium*; Phoenix, AZ; 11-16 October 2015

- *Active and Adaptive Materials Symposium*; New York NY; 22-23 October 2015

- *Materials for the Mitigation of Chemical Hazards Symposium, Pacifichem 2015*; Honolulu, HI; 15-20 December 2015

- *Supramolecular Assemblies at Surfaces: Nanopatterning, Functionality, and Reactivity, Pacificchem 2015*, Honolulu, HI; 15-20 December 2015

- *Gordon Research Conference (GRC) on Electrochemistry subtitled New Directions in Electrochemistry, New Approaches to Electrochemical Problems*; Ventura, CA; 10-15 January 2016

- *2016 CEC Annual Workshop on Electrochemistry*; Austin, TX; 13-14 February 2016

- *56th Sanibel Symposium*; St. Simons, Georgia, 14-19 February 2016

- *Systems for Solar Fuels Generation Utilizing PV and Electrolysis*; Newark, DE; 7-8 March 2016

- *Symposium on Electrochemistry at Solid/Liquid Interfaces*; San Diego, CA; 13-17 March 2016

- *Gride Scale Energy Storage Symposium*; Phoenix, AZ; 28 March - 1 April 2016

- *Young Giants of Nanoscience 2016 Conference*; Hong Kong; 29 May - 6 June 2016

- *2016 Gordon Research Conference on Energetic Materials*; Stowe, VT; 5-10 June 2016

- *Japan-United States Symposium: Polymer Synthesis for a Sustainable Future*; Hokkaido, Japan; 24-28 June 2016
- *2016 Gordon Research Conference on Crystal Engineering*; Stowe, VT; 26 June - 1 July 2016
- *Gordon Research Conference on Molecular Interactions and Dynamics*; Easton, MA; 9-15 July 2016
- *Molecular Rotors, Motors, and Switches*; Telluride, CO; 18-22 July 2016
- *Polymer Composites and High Performance Materials Workshop*; Santa Rosa, CA; 25-28 July 2016
- *Polymers with Sophisticated Branched Structures Symposium*, *Fall 2016 American Chemical Society National Meeting*; Philadelphia PA; 21-25 August 2016

5. Special Programs. In FY16, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded 13 new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These projects constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Ion Transport in Complex Organic Materials. This MURI began in FY10 and was awarded to a team led by Professor Andrew Herring at the Colorado School of Mines. This MURI team is investigating the interplay of chemical processes and membrane morphology in anion exchange.

Ion transport in complex organic materials is essential to many important energy conversion approaches. Unfortunately, ion transport is poorly understood in terms of its relationship to water content, morphology, and chemistry. While a great deal of research has focused on proton exchange membranes, little work has been performed with anion exchange membranes. This MURI team is studying the fundamentals of ion transport by developing new polymer architectures (*e.g.*, polymer membranes) using standard and novel cations. These new polymer architectures and aqueous solutions containing representative cations will serve as a model system for studies of anion transport and its relationship to polymer morphology. In the longer term, the design and synthesis of robust, thin alkali-exchange membranes, combined with an improved understanding of ion exchange gained through the characterization of these membranes, could enable the development of new classes of fuel cells. If the MURI team can characterize the fundamental processes of ion exchange across these polymer membranes, future fuel cells using similar membranes could harness alkali exchange, resulting in inexpensive, durable, and flexible-source power for the Army and commercial use.

2. Peptide and Protein Interactions with Abiotic Surfaces. This MURI began in FY11 and was awarded to a team led by Professor Zhan Chen at the University of Michigan, Ann Arbor. This MURI is exploring the processes that occur at biological/abiological interfaces. This research is co-managed by the Chemical Sciences and Life Sciences Divisions.

The objective of this research is to develop a systematic understanding of biological/abiological interfaces and how to design systems for predicted biological structure and function. The MURI team is using a combination of modeling and experimental techniques to understand the interactions of peptides and proteins covalently immobilized on abiotic surfaces. Specifically, the team will be investigating two peptides and one enzyme, with a variety of surfaces, such as self-assembled monolayers, chemically functionalized liquid crystalline films, and chemical vapor deposited polymers. The immobilized biological species will be characterized to determine not only structure but also activity. The investigators will utilize systematic modifications of the surface to probe the effect of chemical composition, morphology, and hydrophobicity on biological structure and function. The role of water will also be probed to determine how hydration affects not only immobilization, but also structure and

function. Results from this research may ultimately enable the incorporation of nanostructured abiotic/biotic materials in applications such as sensing, catalysis, coatings, drug delivery, prosthetics, and biofilms.

3. High-Resolution Quantum Control of Chemical Reactions. This MURI began in FY12 and was awarded to a team led by Professor David DeMille at Yale University. This MURI is exploring the principles of ultracold molecular reaction, where chemical reactions take place in the sub-millikelvin temperature regime. This research is co-managed by the Chemical Sciences and Physics Divisions.

The study of ultracold molecular reactions, where chemical reactions take place in the sub-millikelvin temperature regime, has emerged as a new field in physics and chemistry. Nanokelvin chemical reactions are radically different than those that occur at "normal" temperatures. Chemical reactions in the ultracold regime can occur across relatively long intermolecular distances, and no longer follow the expected (Boltzmann) energy distribution. The reactions become heavily dependent on nuclear spin orientation, interaction strength, and correlations. These features make them a robust test bed for long-range interacting many-body systems, controlled reactions, and precision measurements.

The objectives of this MURI are to develop a fundamental understanding of the nature of molecular reactions in the nanokelvin temperature regime and to extend the cooling technique previously demonstrated by Professor DeMille[1] (through a previous ARO award) to other molecular candidates. The researchers will focus will be on the implementation of novel and efficient laser cooling techniques of diatomic molecules, and to understand the role of quantum effects, including the role of confined geometries, on molecules that possess vanishingly-small amounts of thermal energy. This research could ultimately lead to new devices or methods that explicitly use quantum effects in chemistry, such as the precision synthesis of mesoscopic samples of novel molecular compounds, new avenues for detection of trace molecules, and a new understanding of combustion and atmospheric chemical reactions.

4. Coherent Effects in Hybrid Nanostructures. This MURI began in FY12 and was awarded to a team led by Professor Naomi Halas at Rice University. This MURI is investigating nanomaterials and how these materials can control the propagation of electromagnetic (EM) energy.

Fundamental research involving metamaterials, quantum dots, plasmonic nanostructures, and other materials systems during the last decade has demonstrated the unique ability to selectively and actively control and attenuate electromagnetic energy from the far infrared (IR) through ultraviolet (UV) regions. The absorption frequency is dependent on shape, size, orientation, and composition of the nanomaterial. The nanoparticles act as antennae that redirect, focus or otherwise re-radiate the incoming energy. Because this is a resonance phenomenon, the media is generally transparent over a broad frequency range, with one or more resonances that absorb at specific frequencies. A goal in the control of the propagation of EM energy is the design of a material that absorbs over a broad frequency range and is transparent at one or more specific frequencies.

The objective of this research is to develop a fundamental understanding of nanomaterials to control the propagation of EM energy, with a particular emphasis on designing and investigating materials that have a broad spectrum absorption with a narrow, selective window of transmission. The MURI team is using a combination of computational, nanoscale fabrication, and characterization techniques to tailor electromagnetic properties for materials in specific, selected regions of the spectrum. The research team is focusing on designing, synthesizing, and combining nanoparticles and nanoparticle-based complexes to yield nanocomplexes exhibiting optimized coherent effects. This research may ultimately enable the design of materials with precisely-positioned transparency or absorbency windows that will impact Army applications in broadband scattering and absorption.

5. Theory and Experiment of Cocrystals: Principles, Synthesis and Properties. This MURI began in FY13 and was awarded to a team led by Professor Adam Matzger of the University of Michigan at Ann Arbor. This MURI team is investigating molecular co-crystal formation and the implications for controlling solid-state behavior. This research is co-managed by the Chemical Sciences and Materials Science Divisions.

The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Co-crystallization has the potential to impact the macro-

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[1] Shuman ES, Barry JF, DeMille D. (2010). Laser cooling of a diatomic molecule. *Nature*. 467:820–823.

scale performance of many materials, ranging from energetic materials, to pharmaceuticals, to non-linear optics. Unfortunately, the dynamics of molecular co-crystal formation is poorly understood. Molecular co-crystals contain two or more neutral molecular components that rely on non-covalent interactions to form a regular arrangement in the solid state. Co-crystals are a unique form of matter, and are not simply the result of mixing two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure 'parent' crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has not been exploited in broader chemistry and materials science research areas. A recent breakthrough discovery demonstrates that co-crystallization can be used to generate novel solid forms of energetic materials.

The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and to use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties. In the long term, a better understanding and control of molecular co-crystallization has the potential to improve the properties of a variety of materials, including: energetic materials, pharmaceuticals, organic semiconductors, ferroelectrics, and non-linear optical materials.

6. Artificial Cells for Novel Synthetic Biology Chassis. This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj at the University of California - San Diego. The goal of this MURI is to understand how biological and biomimetic synthetic cellular elements can be integrated to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways. This research is co-managed with the Life Sciences Division.

The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as chassis for the engineered biological systems and devices. While single-celled organisms are typically used as synthetic biology chassis, the complexity of even these relatively simple organisms presents significant challenges for achieving robust and predictable engineered systems. A potential solution is the development of minimal cells which contain only those genes and biomolecular machinery necessary for basic life. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, and composite microparticles with stable internal compartments. These advances provide the scientific opportunity to explore the integration of biological and biomimetic elements to generate an artificial hybrid cell that for the first time combines the specificity and complexity of biology with the stability and control of synthetic chemistry.

The objective of this MURI is to integrate artificial bioorthogonal membranes with biological elements to create hybrid artificial cells capable of mimicking the form and function of natural cells but with improved control, stability, and simplicity. If successful, these artificial cells will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology that may ultimately enable sense-and-respond systems, drug-delivery platforms, and the cost-effective production of high-value molecules that are toxic to living cells (e.g., alternative fuels, antimicrobial agents).

7. Attosecond Electron Dynamics. This MURI began in FY14 and was awarded to a team led by Professor Stephen Leone at the University of California - Berkeley. The goal of this MURI is to use attosecond light pulses to study the electron dynamics of atoms and small molecules. This research is co-managed with the Physics Division.

Attosecond dynamics is a new field of scientific investigation which allows one to examine dynamics phenomena on the natural timescale of electronic processes in atoms, molecules, and materials. The timescale of microscopic dynamics in quantum systems occur at a timescale about one order of magnitude less than those for less-energetic processes, such as valence electronic transitions in molecules and semi-conductor materials. A recent scientific breakthrough known as double optical gating has lead to the production of broadband laser pulse widths as short as 67 attoseconds, making direct observation of a variety of electronic phenomena possible in real time. Thus, now there exist opportunities to examine a variety of electron-dynamics phenomena that arise from electronic motions in molecules on the attosecond timescale.

The objective of this research is to harness attosecond pulses of electromagnetic energy to probe matter (e.g., atoms, molecules, plasmas) at attosecond time scales for the real-time observation, control, and understanding of electronic motion in atoms, molecules, and materials. If successful, this research may lead to new synthesis methods, such as plasmonically-enhanced catalysis for the direct reduction of CO_2 to create fuels, new schemes and manufacturing methods for solar photovoltaics, nano-catalysts for fuel combustion, and high-density specific impulse propellants.

8. Multistep Catalysis. This MURI began in FY14 and was awarded to a team led by Professor Shelley Minteer at the University of Utah. The goal of this MURI is to enable multi-step chemical reactions through the rational design of architectures that control the spatial and temporal pathways of precursors, intermediates, and products. This research is co-managed with the Materials Science Division.

The Krebs cycle is an exquisite example of a regulated enzyme cascade which biological systems use to precisely control charge and reactant transport to produce energy for the cell. Conversely, man-made systems typically involve a series of conversions with intermediate purification steps to achieve a desired product, with yield losses that compound with each step. The current approach to achieve multi-step reactions in a single reactor is an arbitrary combination of multiple catalysts that is likely to lead to poor yield with unreacted intermediates or byproducts of reactants that have reacted with the incorrect catalysts. Recent breakthroughs in materials synthesis, such as self-assembly and lock-and-key type architectures, offer control of surface arrangement and topology that enable a much more effective approach to achieving multi-step reactions through control of spatial and temporal transport of reactants, electrons, intermediates, and products.

The objective of this research is to establish methodologies for modeling, designing, characterizing, and synthesizing new materials and structures for the design and implementation of multi-step catalysis. In particular, integrated catalytic cascades will be created from different catalytic modalities such that novel scaffolding and architectures are employed to optimize selectivity, electron transfer, diffusion, and overall pathway flux. If successful, this research will provide unique paradigms for exploiting and controlling multistep catalysis with dramatically enhanced efficiency and complexity. In the long term, the results may lead to new energy production and storage technologies.

9. Multi-Scale Responses in Organized Assemblies. This MURI began in FY16 and was awarded to a team led by Professor Sankaran Thayumanavan, at University of Massachusetts - Amherst. The goal of this MURI is to understand how a molecular level detection can be propagated across a macroscopic material to affect a global property change that spans multiple length and time scales, and connecting these multi-scale events to realize signal amplification. This research is co-managed with the Materials Science Division.

Living systems are complex systems capable of receiving and using information, interacting with each other and their environment, and performing specific functions in response to stimuli occurring at multiple length and time scales. These sophisticated, innate behaviors are essential for survival, and can be extremely valuable in non-natural systems. A variety of synthetic systems have been engineered to respond to specific stimuli; however, the dynamics of the chemical and material processes and interactions occurring at multiple length and time scales throughout the signal-propagate-response pathway are inadequately understood to rationally design autonomous, "living" systems. The daunting challenge toward synthetic "living" systems is predictably propagating a molecular level change, generated through the selective sensing of a trigger, into a readily discernible macroscopic change in a material's fundamental properties. This can only be addressed by developing a fundamental understanding of the chemical processes that occur at multi-scale levels – from molecular to nano to macroscopic length scales and from nanoseconds to hours. The inherent complexity involved in connecting these length scales, and the propagation and amplification of the resulting signals, requires a cohesive, multidisciplinary approach.

The integrated research plan led by Professor Thayumanavan is comprehensive and addresses each of the key elements needed to understand the fundamental multi-scale responses of adaptive systems occurring across length and time scales. The research is exploiting a variety of material platforms/approaches, including liquid crystal orientation, responsive amphiphiles, depolymerization, and biological/abiological composites with non-equilibrium molecular release to address propagation and amplification at multiple length scales. Each system approach is innovative, well-formulated, and focused on a complete understanding of the basic research principles controlling each approach.   A variety of triggers will be considered throughout the effort including pH, temperature, redox, light, and enzymes.   A key part of this effort is the ability to monitor dynamic changes

during the cooperative reorganization processes at the interface, and this is addressed by integration of novel characterization techniques such as in situ liquid cell transmission electron microscopy.   If successful, this fundamental research may ultimately enable Army-relevant technologies in stimuli-responsive systems such as self-decontaminating materials, controlled release for hazardous materials management or drug delivery, and responsive systems for self-healing and smart materials.

10. Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery. This MURI began in FY16 and was awarded to a team led by Professor Michael Jewett at Northwestern University – Evanston. The goal of this MURI is to engineer the translation machinery to accept and polymerize non-biological monomers in a sequence-defined manner using non-traditional chain growth polycondensation chemistries (beyond amide and ester linkages). This research is co-managed by the Chemical Sciences (lead) and Life Sciences Divisions.

Employing only four nucleotides and twenty amino acids, a plethora of biopolymers (e.g., proteins, DNA) with precisely-defined building block sequence gives these materials the ability to fold into higher-ordered structures capable of performing a variety of advanced functions such as information storage, self-replication, and signal transduction. The ability to extend comparable molecular-level sequence control to synthetic polymers, which have a much wider range of monomeric building blocks, has many scientific and technological implications, as it would enable precise control over structure-property relationships. Recent work has demonstrated that altering the sequence of short conjugated phenylene-vinylene oligomers can significantly modulate both electronic and optical properties. While greater complexity in function is anticipated for longer chain sequence-defined polymers, chemical routes to their synthesis have remained elusive. Conversely, biology synthesizes long sequence-defined polymers with extremely high efficiency and accuracy by employing templates to provide sequence information. More specifically, the ribosome, the workhorse of the translation machinery, is very adept at sequence-defined polymer synthesis through the successive condensation of amino acids (monomers), but primarily performs a single type of chemistry—amide bond formation via a chain-growth condensation polymerization. Co-opting the natural translation machinery to accept non-biological monomers is an attractive approach to synthesize non-biological polymers with the sequence control of biology. However, this approach is limited by cell viability constraints; thus, in vitro engineering of the translation machinery may offer unprecedented freedom of design to modify and control ribosome chemistry.

The objective of this research is to engineer and repurpose the translation apparatus (including the ribosome and the associated factors needed for polymerization) to produce new classes of sequence-defined polymers. In the long term, this research may enable a broad range of disruptive technologies having significant impact on DoD capabilities. Sequence control at the atomic level will give the greatest possible control over the emergent, macroscopic behavior of oligomers and polymers, leading to new advanced personal protective gear, sophisticated electronics, fuel cells, advanced solar cells, and nanofabrication, which are all key to the protection and performance of soldiers.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES. The Division managed eight new-start SBIR contracts in FY16, in addition to managing active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY16 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES. In FY16, the Division managed seven new-start STTR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of STTR topics published in FY16 and a list of prior-year topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY16, the Division managed five new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. Although PECASE nominations were submitted by this Division in FY16, selections had not yet been made by OSD nor announced by the White House. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY16, the Division managed five new DURIP projects, totaling $1.0 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. University Affiliated Research Center (UARC): Army Institute for Soldier Nanotechnologies (AISN)

The AISN, located at the Massachusetts Institute of Technology (MIT), carries out fundamental, multidisciplinary, nanoscience research that is relevant to the Soldier. Nanoscience research creates opportunities for new materials, properties, and phenomena as material properties (*e.g.*, color, strength, conductivity) become size dependent below a critical length scale of about 100 nanometers. The research performed at the AISN falls into three Strategic Research Areas (SRAs): (i) Lightweight, Multifunctional Nanostructured Materials (ii) Soldier Medicine, and (iii) Blast and Ballistic Threats. Each SRA is further divided into research themes. Detailed descriptions of each SRA and its corresponding themes are available at the AISN program website (http://mit.edu/isn/research/index.html).

In FY16, the AISN supported 27 faculty, 65 graduate students, and 25 postdoctoral fellows across 14 departments at MIT. The AISN program is unique in that it currently has 10 industrial partners positioned to receive promising technical results and work to bring new products and capabilities to the Soldier, as well as a mechanism for additional industry partners to join and leave the Institute, depending on needs and activities. A U.S. Army Technical Assessment Board and an Executive Steering Board biannually review the AISN research portfolio, assessing the goals of the various projects and research results. The AISN and its industry partners are well-situated to perform basic and applied research in response to Soldier needs now and in the future. A total of $7.7 million of program funds was allocated to the AISN in FY16, which was the fourth year of a contract that was renewed in FY12 for a five-year period. Of these FY16 funds, $4.7 million was allocated for 6.1-basic research and $2.0 million was allocated for six applied-research projects.

I. DARPA Agnostic Compact Demilitarization of Chemical Agents (ACDC) Program

DARPA's Agnostic Compact Demilitarization of Chemical Agents (ACDC) program is exploring new technologies for neutralization of bulk stores of chemical warfare agents (CWAs) and organic precursors at or near the site of storage. ACDC is developing and demonstrating the technologies needed to construct a transportable, prototype system that converts organic compounds into constitutive carbon/nitrogen/phosphorous/ sulfur oxides and stable alkali or alkaline earth metal salts, or another demonstrated safe form. A final ACDC system would feature chemistries for agent destruction and sequestration of halogens and other components

using locally available resources. ARO is providing subject matter exptertise and an ARO program manager is serving as the COR on the awarded efforts.

J. DARPA Make-It Program

The DARPA Make-It program aims to address these challenges by developing technologies to accelerate chemical discovery and production beyond conventional batch-based capabilities by exploiting continuous synthetic approaches. The goal of Make-It is to develop a fully automated chemical synthesizer that can produce, purify, characterize and scale a wide range of small molecules. Make-It systems would likely include components for knowledge-based computational tools for reaction pathway prediction; algorithms for automation and process control; and interconnected fluidic modules for continuous synthesis, in-line characterization, purification and formulation. If realized, such a system would not only speed the pace of chemical innovation and small-molecule manufacturing, but would also provide an accessible chemical synthesis platform for non-specialists. ARO is providing subject matter exptertise and an ARO program manager is serving as the COR on the awarded efforts.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Chemical Sciences Division.

A. Photocatalysis at TiO₂-Supported Au Nanoparticles
Professor John Morris, Virginia Tech, Single Investigator Award

The goal of this research is to formulate a mechanistic understanding of activation and charge transfer that govern thermal- and photocatalytic chemistry on the surface of TiO_2-supported Au particles. Previous work provided insight into the thermal- versus photooxidation mechanisms of methanol on Au/TiO_2.

In FY16, the research team shifted their investigation to propene adsorption and oxidation on Au/TiO_2 catalysts (see FIGURE 1). Using a combination of DFT calculations and Fourier transform infrared (FTIR) spectroscopy data, two distinct propene-surface binding motifs were identified: one corresponding to propene bound to the surface through a π-interaction at TiO_2 sites remote from the Au particles; and the other corresponding to a (πσ)-interaction at a single atomic Au site. Temperature programmed desorption and calculated binding enthalpies for the minimum energy configurations revealed that the propene-Au interaction has a stronger binding energy relative to the propene-TiO_2 interaction (see FIGURE 2). Upon coordination to Au, the double bond of propene weakens and elongates, a critical first step in the activation and epoxidation to form propene oxide. The next stage of research will focus on elucidating the role of photonic excitations in driving the oxidation of propene and other small organic compounds.
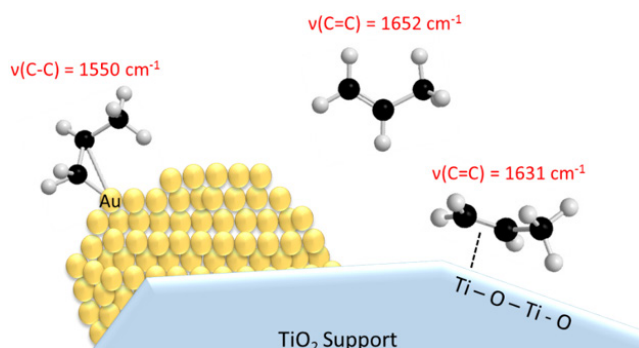
FIGURE 1
Adsorption of propene onto activated Au/TiO₂.
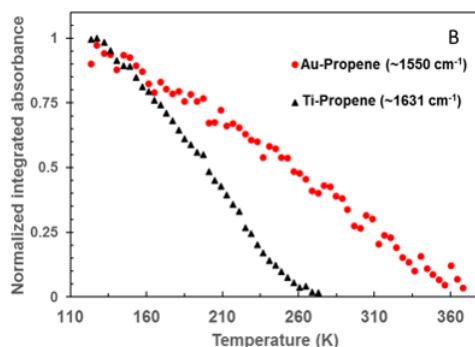
FIGURE 2
Temperature programmed desorption of propene on Au/TiO₂. Integrated absorbance of the 1550 and 1630 cm⁻¹ IR bands at specific temperatures throughout the temperature ramp.

B. Dynamic Control of Self-Organized Assemblies Using Near-Infrared and Visible Light Activated Azo-BF₂ Switches
Professor Ivan Aprahamian, Dartmouth College, Single Investigator Award

The goal of this research is to decipher the fundamental factors that control the photophysical properties of BF_2-azo switches and implement the switches as chiral dopants that effectively and efficiently control the optical properties of liquid crystals. Previous research on a series of azo-BF_2 complexes demonstrated that a range of Z to E isomerization rates (seconds to hours) could be obtained using visible and near IR light sources. Addition of electron donating *para*-substituents on the azo-BF_2 complexes red-shifted the activation wavelength of the complexes but also resulted in a dramatic shortening of the isomerization half-lives.

In FY16, to tailor the same red-shift effect without negatively impacting the isomerization half-life, the research team investigated expansion of the π-system from a quinolinyl group to a phenanthridinyl group (see FIGURE 3). The modified compound, **1**, was irradiated with visible light and demonstrated a small red-shift in activation wavelength relative to the parent compound. More importantly, the system forms supramolecular aggregates in solution which drastically modulates the Z to E thermal isomerization rate by up to a factor of 1800 (from seconds to days). The thermal Z to E isomerization rates is linearly dependent on the degree of aggregation in solution: the higher the concentration, the larger aggregates in solution, and the slower the isomerization rate (see FIGURE 4). This unprecedented discovery is a promising approach to control the thermal properties of photochromic compounds.
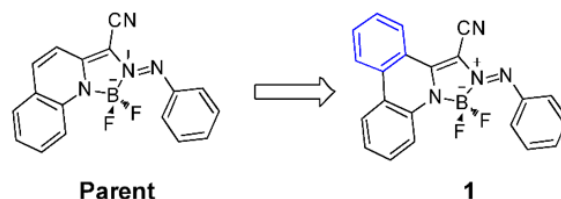
Parent **1**

FIGURE 3
Structure of parent azo-BF_2 complex and compound **1**.
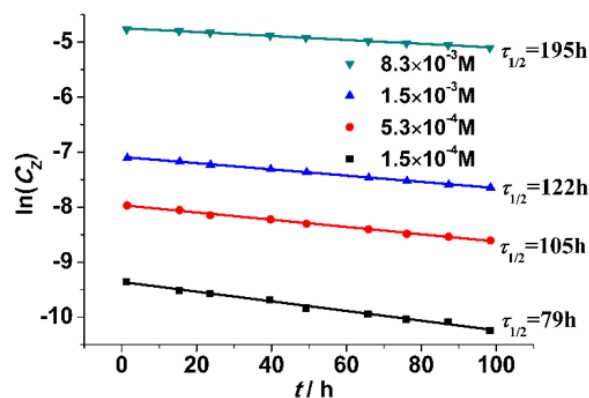
FIGURE 4
The concentration dependent Z to E isomerization half-lives of **1** in CD_2Cl_2 at room temperature.

C. Highly Vibrationally Excited (v ≥ 4) H₂ Molecules by Stark-induced Adiabatic Raman Passage
Professors R. Zare and N. Mukherhee, Stanford University, Single Investigator and DURIP Awards

The investigators have previously shown preparation of an ensemble of vibrationally excited ($v = 1$) diatomic hydrogen molecules in a supersonically espanded molecular beam using a coherent Raman method that they term as Stark-induced adiabatic Raman passage (SARP). The method should have general applicability, but, until now it has only been shown for the case of HD ($v = 0$ to $v = 1$). To further demonstrate the utility of SARP, the investigators have completed experiments in which one hundred percent of the population of HD ($v = 0$, $J = $

0) in a supersonically expanded molecular beam is transferred to HD ($v = 4$, $J = 0$). This was achieved with a sequence of partially overlapping nanosecond pump (355 nm) and Stokes (680 nm) single-mode laser pulses of unequal intensities (see FIGURE 5). By comparing the experimental data with theoretical calculations, the investigators draw two important conclusions: (1) using SARP, a large population (more than 10^{10} molecules per laser pulse) is prepared in the ($v = 4$, $J = 0$) level of HD, and (2) the polarizability of the Raman overtone transition ($v = 0$ to $v = 4$) is only about five times smaller than that for the ($v = 0$ to $v = 1$) fundamental Raman transition. Additionally, the SARP process selects a specific rotational level in the vibrational manifold and can prepare one or a phased linear combination of magnetic sublevels (M states) within the selected vibrational-rotational level. This capability of preparing selected, highly excited vibrational levels of molecules undercollision-free conditions opens new opportunities for fundamental reactive or non-reactive scattering experiments. It is likely that SARP will be a key method for future landmark experiments of state-selected chemical reactions.
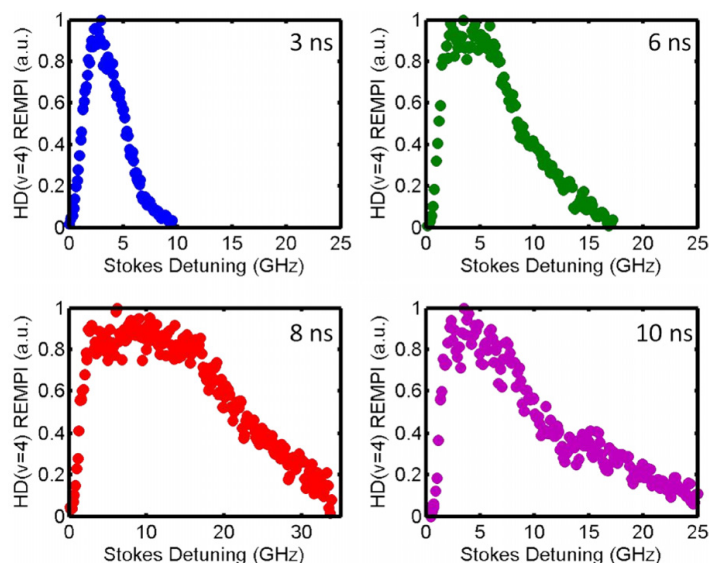
FIGURE 5

Experimental (2+1) REMPI signal from SARP excited X $^1\Sigma^+_g$ HD ($v = 4$, $J = 0$) as a function of Stokes frequency. Pump fluence is approximately 12 J/mm^2 and Stokes fluence is approximately 1.3 J/mm^2 and detuning for the pump to Stokes delays of 3 ns, 6 ns, 8 ns, and 10 ns.

D. Integrated Multi-Scale Approach For Understanding Ion Transport In Complex Heterogeneous Organic Materials
Professors Andrew Herring (lead PI), Colorado School of Mines, MURI Award

The objective of this research is to develop thin robust anion conducting polymer electrolyte membranes (PEM) from the ground up using theory, directed polymer synthesis and advanced analytical tools. This MURI team is led by Professor Andrew Herring and includes the co-PIs Daniel Knauss at the Colorado School of Mines, Professor E. Bryan Coughlin at the University of Massachusetts - Amherst, Professor Matthew Liberatorre at the University of Toledo, Professors Gregory Voth and Thomas A. Witten at the University of Chicago, and Professor Vito Di Noto at the University of Padova.

By definition a PEM that is an anion conductor must be functionalized with organic cations. Even the simplest organic cation, trimethyl benzyl ammonium has a strong dipole. These dipoles have a tendency to line up head to tail causing clustering of the cations in the PEM. This makes the issues of designing a high performance PEM much more complex, not only will increasing the ion exchange capacity (IEC) of the material result in uncontrollable swelling, but as the concentration of cations increases they tend to cluster and no matter how many cationic groups are added to a random polymer the ionic conductivity will not increase. To investigate this phenoma and to work out a solution the MURI team made a large series of polymers consisting of polyisoprene (PI) and polyvinylbenzyltrimethyl ammonium (PVBTMA), (see FIGURE 6)
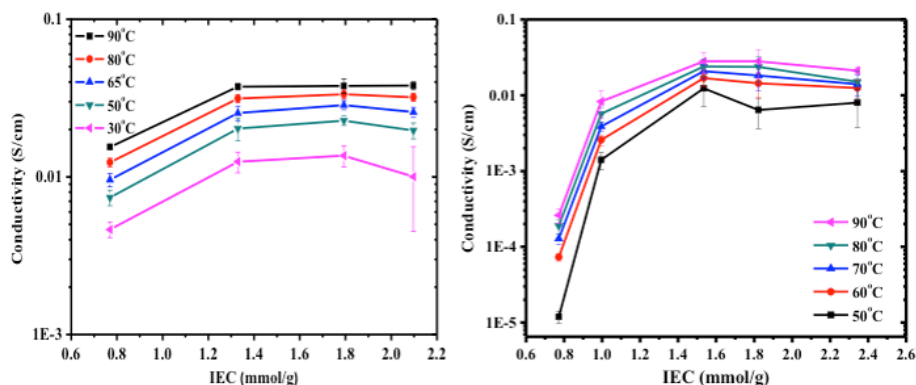
FIGURE 6

Analysis of PI and PVBTMA-containing polymers. Bromide conductivity for a PI-*ran*-PVBTMA polymer (left) and for a PI-*b*-PVBTMA polymer (right) at 95% RH. Note that for a random polymer there was no increase in bromide conductivity after an IEC of 1.3. This was improved by taking the same polymer composition and making a block co-polymer, where the conductivity threshold now occurs at a IEC of 1.6.

The team found that by using polymer cross-linking to lock the morphology in place further performance improvements could be made. The idea was to control water uptake and lock the morphology via cross-linking, either thermally or by photochemical methods. Photo-crosslinking offers several advantages over thermal-crosslinking: (i) ambient reaction temperatures greatly reduce possible side reactions, (ii) efficient crosslinking is achieved within seconds to minutes, and (iii) the application area is readily adjustable, thus larger and thinner membranes can be prepared. Photoinduced radical mediated thiolene chemistry has been widely used to obtain cross-linked networks and to functionalize polymers. Additionally the cross-linker can be chosen to add hydrophilicity or hydrophobicity to the polymer.

Broad band electric spectroscopy (BES) is a powerful tool for understanding the mechanical transitions and polarization events in PEMs. Many of the BES studies of anion conducting PEMs were extremely complex and often showed a transition between 30 - 60°C attributed to clustering of the cationic dipoles in the PEM. The researchers found that in a BES of a PI-*b*-P[VBTMA]OH⁻ polymer, the conductivity (σ) rises rapidly at the melting point of water, showing a dependence of conductivity on liquid water, however it falls rapidly a few 10's of degrees higher in temperature (see FIGURE 7). This fall in conductivity was assigned to T_δ, a disorder/order transition where the cations have enough energy to overcome their spacing on the polymer backbone and cluster, dramatically lowering the local anionic conductivity. The same transition is observed in small angle x-ray scattering (clusters around 30 nm) and mechanical data implying that it could also lead to a weakening of the material in applications where it is cycled. The BES of a photo cross-linked PI-*ran*-P[VBTMA] Cl⁻ polymer was found to be unusually simple when compared to similar materials. One beta relaxation (due to the cationic side chains) and two modes of conductivity, are observed, in contrast with the complex BES behavior observed for the PI-*b*-P[VBTMA] polymer. Again a large increase in conductivity at 273K is observed as the water in the film melts and the water-mediated conductivity dominates. Interestingly the order disorder transition seen in non-cross-linked analogues is not observed, and the conductivity plateaus and dominates the BES spectrum to >100°C. This material, which is currently being investigated, is a scalable polymer system that can be rapidly cross-linked and in the future functionalized with more chemically stable advanced cations.
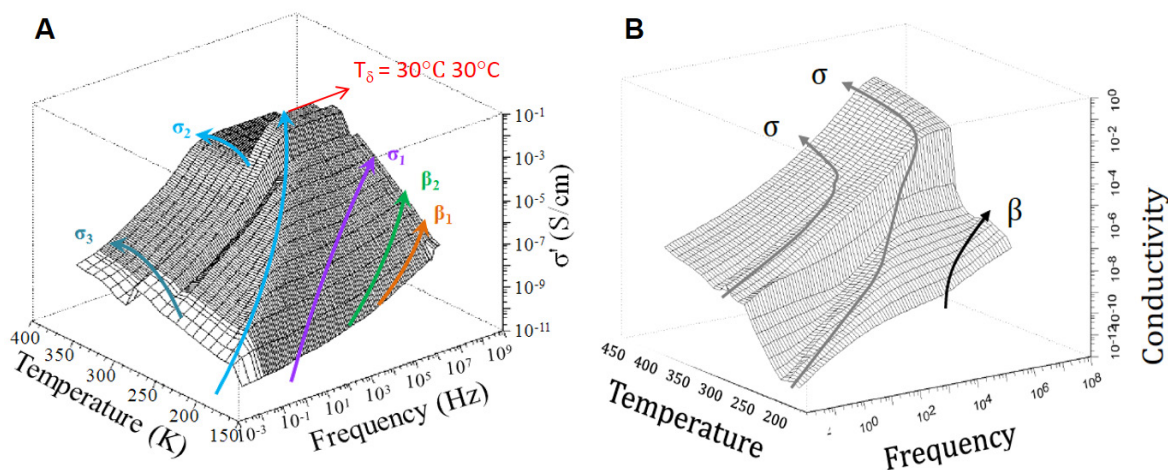
FIGURE 7

Broad band electric spectrums of (**A**) PI-b-P[VBTMA] OH⁻ and (**B**) photo-crosslinked PI-ran-P[VBTMA] Cl⁻ polymer.

E. Understanding the Novel Stimuli Responsive Transport Properties of Multifunctional, Nanostructured Block Polymer Membranes
Professor William Phillips, Notre Dame University, Young Investigator Award

The objective of this research is to develop systematic structure-property-performance relationships for the design of self-assembled block polymer membranes. Such membranes have the potential to render a novel membrane platform that possesses require high throughput, high surface area, a well-defined pore size, and varying material functionality.

In FY16, research efforts resulted in significant progress on three fronts related to this overarching objective. First, the research team began identifying the molecular interactions that generate a unique, long-lived hysteretic response to solution pH in block polymer membranes. The enhanced understanding of the polymer physics governing the response of a nanoscale polymeric material that has a memory of its previous environment provides insight into the design and manipulation of next-generation sensors and gating materials. Second, the self-assembly and non-solvent induced phase separation (SNIPS) fabrication technique was integrated with the dip coating archetype in order to produce high performance block polymer membranes in the hollow fiber configuration. The development of block polymer membranes in the hollow fiber geometry is crucial to expanding their utility to a broader range of applications because, when applied in full-scale modules, hollow fiber membranes are able to provide higher packing densities (i.e., active surface area per module volume) and, in turn, a higher throughput of processed solution. Finally, the chemical versatility purposefully built into this novel block polymer membrane platform was used to affix heavy metal binding ligands within the nanopores of the membranes and demonstrated the use of these functionalized thin films as high capacity adsorbers in water treatment applications (see FIGURE 8).

FIGURE 8

Block polymer copper-selective membrane used to affix heavy metal binding ligands within nanopores.

While the nanopore chemistry is molecular engineered for the removal of heavy metal pollution from water in the team's initial efforts, the functional advantages of the materials demonstrated could easily be extended to other recalcitrant pollutants or applications beyond the environmental science and engineering sphere (e.g., as a

high capacity urea adsorber for dialysis in biomedical applications). These initial results grounded in fundamental polymer science and engineering are promising. As such, this research presents an opportunity to make significant progress toward elucidating the structure-response relationships for block polymer membranes that offer enhanced throughput and improved selectivity in traditional and emerging membrane applications.

F. Novel Thermal Radiation Management Using Advanced Photonic Crystals
Professors Ivan Celanovic, John Joannopoulos, and Marin Soljacic, Massachusetts Institute of Technology, AISN (UARC)

This research, led by investigators at the Army Insitiute for Soldier Nanotechnologies (AISN), aims to expand the frontiers of high-temperature nanophotonics, explore new physical phenomena that enable unprecedented control of thermal radiation and radiative heat transfer at the nanoscale and at very high temperatures (>800°C), and demonstrate novel materials, devices, and system level applications ranging from chipscale MEMS based thermophotovoltaics (TPV), small-scale radioisotope power sources, all the way to nonconventional infrared (IR) light sources and room-temperature IR detectors.

In FY16, the research team has demonstrated how a plain incandescent tungsten filament (3,000 K) surrounded by a cold-side nanophotonic interference system optimized to reflect infrared light and transmit visible light for a wide range of angles could become a light source that reaches luminous efficiencies (~40%) surpassing existing lighting technologies, and nearing a limit for lighting applications (see FIGURE 9). The research team experimentally demonstrated a proof-of-principle incandescent emitter with efficiency approaching that of commercial fluorescent or light-emitting diode bulbs, but with exceptional reproduction of colors and scalable power. The ability to tailor the emission spectrum of high-temperature sources may find applications in thermophotovoltaic energy conversion and lighting.
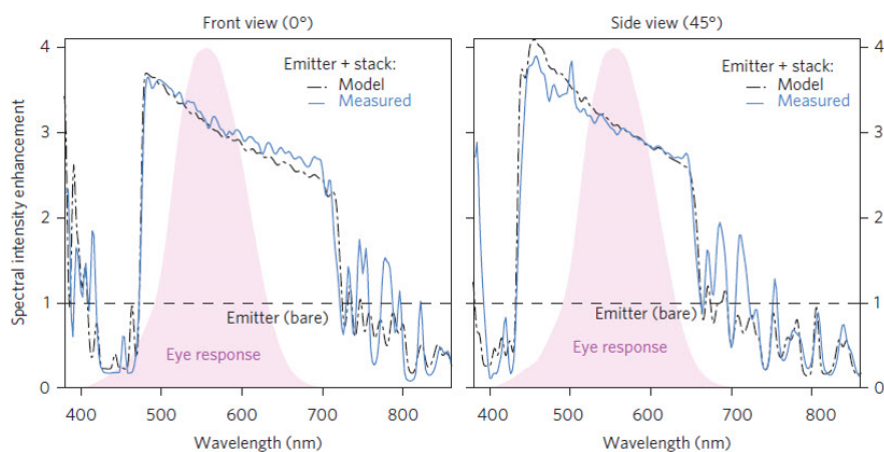

FIGURE 9

Experimental demonstration of thermal emission tailoring. Measured (blue, solid) and modelled (grey, dashed-dot) spectral intensity of the combined emitter-tailoring-structure system ('Emitter + stack') normalized to the intensity of the plain emitter (black, dashed) that consumes the same amount of power. The fabricated structure consists of 90 layers and is made of two materials (SiO_2 and Ta_2O_5) deposited on a silica substrate. The spectrum is measured at 0° (front view) and 45° (side view). The sensitivity of the human eye (luminosity function) is shown in shaded purple. For the same amount of input power, the luminous flux is 3.07 (2.90) times enhanced at 0° (45°) compared with that of a plain emitter.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Interfacial Damage and Water Sensor for Composites Using a Rhodamine Spirolactam
Investigator: Jeffrey W. Gilman, NIST, STIR Award
Recipient: Owens Corning

The goal of this research was to use mechanophores and single-molecule fluorescence microscopy (SMFM) to create super-resolution sensors in the interphase in polymer nanocomposites to see if this spectroscopic technique can be applied to heterogeneous polymeric materials. The ARO-funded investigators successfully developed a rhodamine spirolactam mechanophore which is easily incorporated at a composite interface, or in the matrix, using a simple 1 or 2 step procedure. DFT studies revealed that the mechanophore is stronger than other spyropyran-based mecnahophores, is thermally-reversible, has sufficient quantum yield and photostability to enable fluorescence lifetime imaging of damage in mechanically stressed composites (see FIGURE 10). It was also discovered that this fluorogenic probe can also work as a water sensor in composites. These mechanophores transitioned to Owens Corning, which then evaluate these two probe systems using fluorescence imaging to develop tougher, lightweight, durable composites. These studies began in FY16 as a two-year cooperative research agreement with NIST.
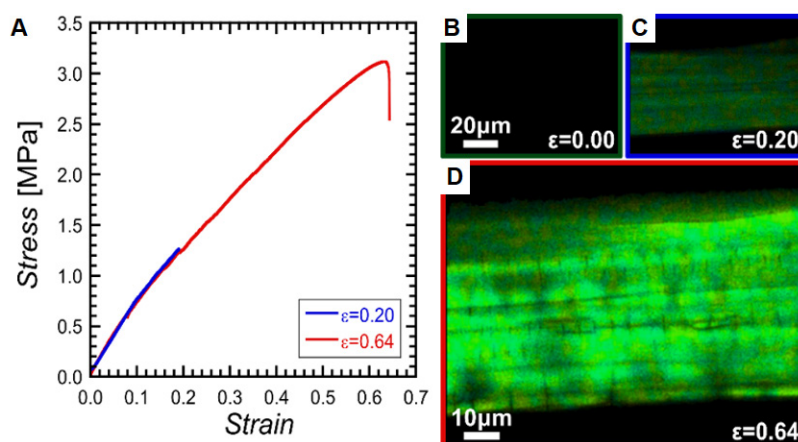
FIGURE 10

Activation of MP at the interface of a single fiber bundle silk epoxy by mechanical deformation. (A) Uniaxial tensile response of single fiber bundle composites after the application of moderate strain ($\varepsilon = 0.20$) and critical strain ($\varepsilon = 0.64$). (B-D) Corresponding TP-FLIM images of fiber composites. (B) Prior to deformation, minimal fluorescence is observed. (C) At $\varepsilon = 0.20$, a uniform, low intensity fluorescence is observed with minimal visible damage to the fiber surface. (D) At $\varepsilon = 0.64$, the sample fractures, the fluorescence intensity is heterogeneous but overall brighter than at moderate strain, and numerous microcracks can be seen on the surface of the fiber bundle.

B. Electrode/Electrolyte Interface of All Garnet Solid State Li-Ion Batteries
Investigator: Professor Chunsheng Wang, University of Maryland College Park, STIR Award
Recipient: Ceramatec, Inc.

The objective of Professor Wang's research is to understand origins of the large interfacial resistance between electrode and $Li_7La_3Zr_2O_{12}$ (LLZO) solid electrolyte with the aim to develop a safe, high-performance all-solid-state lithium battery. Research efforts in FY16 focused on reducing the interface resistance between the $LiCoO_2$ (LCO) cathode and LLZO solid electrolyte. Professor Wang and his team developed an innovative approach to reduce the huge LCO/LLZO interfacial resistance in the Li/LCO solid state Li batteries by creating an artificial

Li_2CO_3 solid electrolyte interphase between LCO cathode and LLZO electrolyte. A superior LCO/LLZO interface was achieved with the simultaneous improvements in the interfacial contact, electrochemical and chemical stability, ionic conductivity and mechanical strength, leading to significant improvement in electrochemical performance of all ceramic Li/LLZO/LCO cells. The interphase-engineered Li/LLZO/LCO cells delivered a large reversible capacity (106 mAh/g) for 40 cycles with a high-rate capability (up to 1 C) at 100 °C, representing the best performance of the all ceramic LLZO-based SSBs reported to date (see FIGURE 11). It is a major breakthrough towards the development of safe, high-performance all-solid-state lithium batteries. These results have transitioned to Ceramatec, Inc., which is evaluating the discoveries for potential commercialization.
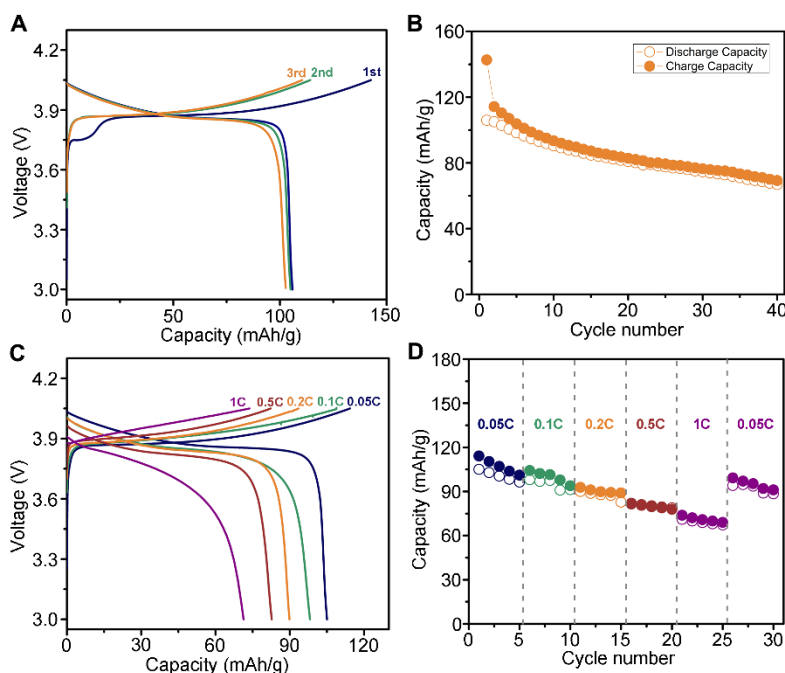
FIGURE 11
Electrochemical performances of the interphase-engineered Li/LLZO/LiCoO₂ all ceramic cell.
Charge/discharge profiles in the first three cycles (**A**) and cycling stability (**B**) of Li/LLZO/LiCoO₂ all ceramic cell at 0.05 C; The charge/discharge behavior (**C**) and capacity (**D**) of Li/LLZO/LiCoO₂ all ceramic cell at different rates from 0.05 C to 1 C.

C. Li₂S-Carbon Composite Technology for Li and Li Ion Batteries
*Investigator: Professor Gleb Yushin, Georgia Institute of Technology, Single Investigator Award
Recipient: Sila Nanotechnologies, Inc.*

The goal of this research is to investigate hierarchical nanocomposite particle-shell architecture of Li_2S cathode, which offers the multi-level protection against damages within protective coatings of particles. Low-cost sulfur-based cathodes offer an order of magnitude higher gravimetric capacity compared to traditionally used lithium metal oxide cathodes and additionally allow for significantly enhanced safety features. Their common limitations include rapid degradation, low capacity utilization and low rate performance. The unique architecture of the Li_2S cathode not only drastically reduces internal stresses within outer shells, but also allows one to achieve high capacity utilization of insulative Li_2S for a relatively large size of the composite particles (see FIGURE 12). At a moderate temperature of 45 °C the cell with hierarchical Li_2S-based active particles showed reversible capacities of 1020-1310 mAhgs^{-1} at very high (for this chemistry) C rates of 5C-1C, respectively, which are even higher than the previously reported graphene/CNT/S nanocomposites. Such remarkable rate performance and small hysteresis are due not only to small sizes of Li_2S nanocrystals and high electrical conductivity of carbon matrix, but also to prevention of polysulfide dissolution and the related lack of resistive layers build-up on the surface of both electrodes. Virtually no degradation could be detected within 100-600 cycles. The proposed particle

architecture and general synthesis route could be effectively utilized for building electrochemical cells with a variety of other conversion-type cathode materials, which undergo significant volume changes during cycling and suffer from undesirable interactions with electrolytes and low conductivity. These results have transitioned to Sila Nanotechnologies, Inc., which is evaluating surface-protected hierarchical Li_2S material technology for commercial applications in ultra-high specific energy batteries.
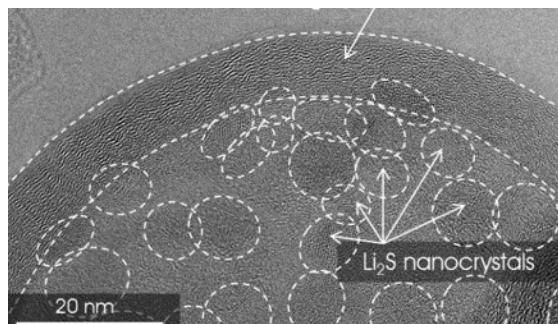
FIGURE 12

TEM characterization of the hierarchical composite Li_2S-C samples (graphitic outer shell indicated by top arrow).

D. Heat Engines Using a Non-Ideal Fluid Model with Higher Efficiencies Vs Ideal Gas Model
Investigator: Ilki Kim, North Carolina A&T State University, HBCU Award
Recipients: ARL Vehicle Technology Directorate (ARL-VTD), NASA Glenn Research Center

The objective of the originating research is to determine how scaling down into the nanoscale affects the ability to define thermodynamic variables in electrochemical experiments, as well as building and controlling thermodynamic machines. In FY16, Professor Kim's team found that a real engine model can go beyond its ideal-gas counterpart in efficiency, whereas as well-known, the maximum Carnot efficiency is the same for both ideal and non-ideal gas engines. Interestingly, the team found that the higher the non-ideality is, the higher efficiency tends to be found, especially in the low-temperature regime, but with more shrinkage in the range of physically allowed compression ratio, determined by the Carnot upper bound, namely, the Second Law of thermodynamics. Specifically, the researchers considered both Otto and Diesel heat engine cycles running upon the working substances modeled by the van der Waals fluid as a simple non-ideal gas model. This advance was noteworthy when compared to data that the actual non-ideal gas in thermal processes of the typical internal combustion engines of industry would produce, for a given internal pressure, the lower internal temperature (as a measure of the available thermal exergy) than its counterpart calculated from the ideal gas model. The team's findings imply that in addition to the engine architectures and bath temperatures, the properties of working substances should also be taken into consideration in the performance study of heat engines, the theoretical model aspects of which have not sufficiently been discussed so far. These studies transitioned to ARL-VTD and the NASA Glenn Research Center for further study to explore potential applications in other non-ideal fluid models and for the efficient management of thermal and mechanical energy at macro level, such as in the optimal design of next-generation heat engines for ground and air vehicles.

E. Determination Of Oxygen And Hydrogen Mass Transfer Coefficients In PEMFC GDE And Their Separation Into Gas And Electrolyte Contributions
Investigators: T. V. Reshetenko and J. St-Pierre, Hawaii Natural Energy Institute, University of Hawaii
Recipient: Industry

The objective of this research is to develop and validate a method of determination of reactant mass transfer coefficients in proton exchange membrane fuel cells (PEMFCs). The method is based on limiting current distribution mathematical mode and variations in oxygen/hydrogen diluent molecular weight. In FY16 the reproducibility of two methods based on local and average limiting current models was demonstrated for oxygen stream. The separation of the oxygen mass transfer coefficient into gas phase molecular diffusion and a combination of diffusion in fine pores (Knudsen diffusion) and the ionomer/water films was simplified by decreasing the number of gas diluents from 9 to 3 (He, N_2 and C_3F_8) reducing cost and measurement time.

Analytical physical impedance models (one-dimensional and quasi-two-dimensional) were validated to determine transport parameters. These results have transitioned to Nuvera Inc. and 3M, that will collaborate by validating the methodology for different flow field designs and electrode structures. If successful, the research will provide a tool for diagnostics of mass transport limitations in PEMFC and a guidance for improvement of membrane/electrode assembly design, decreasing of fuel cell size in applications with volume restrictions and support cost reduction efforts.

F. Cobalt-free and Uranium-free Nanocrystalline Alloy
Investigator: Professor Chris Schuh, AISN (UARC)
Recipient: Veloxint, Corp

AISN researchers, in collaboration with ARL and ARDEC scientists have discovered a nanocrystalline metal alloy with extraordinary properties (e.g. >200% stronger) that is free of both carcinogenic cobalt and hazardous depleted Uranium. Initial field tests show promising performance with potential military applications that include penetrators, armor, and lightweight aerospace or vehicle components. These studies were published in FY16 by the AISN, ARL, and ARDEC researchers.[2] The new alloy has transitioned to ARL-WMRD and ARDEC for further study to determine if the material can provide a significant weight reduction for a variety of applications that are being pursued such as carbide replacements for small and medium caliber penetrators and related high-density metals products.

G. Shape Memory Alloy for Potential Electronics Applications
Investigators: Professors Chris Schuh and Raul Radovitzky, AISN (UARC)
Recipient: Kinalco, Inc.

Army sponsored AISN researchers have developed a continuous oligocrystalline shape memory alloy (SMA) wire produced by melt spinning in the AISN laboratory. AISN researchers have discovered the critical physics that permit continuous casting of super meter scale Cu-based SMA microfibers directly into a desirable oligocrystalline microstructure. Previously, SMA oligocrystals were produced in a 2-step process that involved a grain growth heat treatment. The new discovery permits a single-step production method that leads to a favorable texture as well as achieving large superelastic strains. Results from the new method may lead to a manufacturing route for inexpensive smart fabrics and textiles. This AISN work on superelastic alloy research has transitioned to the startup company Kinalco, Inc., to produce oligocrystalline fibers and wires for a variety of applications that range from orthodontics and electronics to Army-relevant protective materials.

H. Integrated Multi-Scale Approach For Understanding Ion Transport In Complex Heterogeneous Organic Materials
Investigators: Professor Andrew Herring, Colorado School of Mines, MURI Award
Recipient: ProtonOnSite

This MURI team is studying the fundamentals of ion transport by developing new polymer architectures (*e.g.*, polymer membranes) using standard and novel cations. These new polymer architectures and aqueous solutions containing representative cations will serve as a model system for studies of anion transport and its relationship to polymer morphology. In the longer term, this research may enable new classes of fuel cells.

Professor Herring and co-PI Professor E. Coughlin at the University of Massachusetts - Amherst, recently discovered anion exchange membranes with very desirable properties. The new polymers have high hydroxide conductivity and dramatically improved stability, and also have easily scalable synthetic routes and are processable into thin films. The base polymer has a triblock hydrocarbon structure that is prepared in only two steps. This material is also easily cross-linked by methods developed at U. Mass that enable the tuning of its

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[2] Corderoa ZC, Carpenterb RR, Schuha CA, Schusterc BE. (2016). Sub-scale ballistic testing of an ultrafine grained tungsten alloy into concrete targets. *International Journal of Impact Engineering*. 91: 1-5

mechanical properties. The key is to functionalize the material with a methyl pyrrolidinium cation that has recently been identified as having very high stability. Results revealed that a polymer functionalized with this cation has the highest stability in accelerated testing, compared with the 5 carbon ring methyl piperidenium cation and strikingly the first generation trimethyl-ammmonium benzyly cation and the bulky phosphonium cation (see FIGURE 13). These results are also borne out in conductivity testing at 95% RH where the triblock polymer with the methyl pyrrolidinium cation and modest IEC has the highest conductivity approaching 0.1 S cm-1 at 80°C. The swelling from water vapor is minimal and even from liquid water is half that of a typical proton exchange membrane. The materials are tough due to the nature of the cross linking that occurs during thermal processing and the films can be made as thin as 20 µm. Anion exchange membranes have the potential to completely change direct polymer electrolyte membrane fuel cells, electrolysis for hydrogen production or for the production of electrofuels such as ammonia as the catalysts are non-precious metals. These results have transitioned to ProtonOnSite, which will evaluate the membranes for commercial applications in electrolyzers.
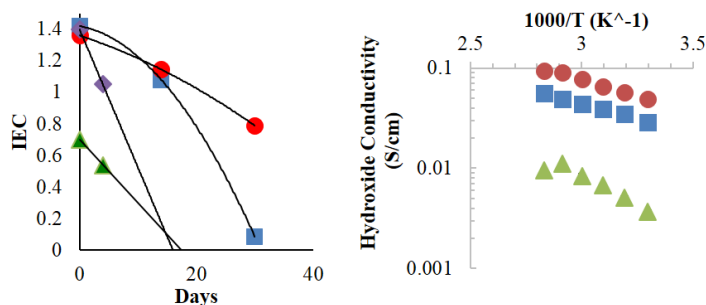
FIGURE 13

Stability data for the triblock polymer in 1M KOH at 80 °C, and hydroxide conductivity data at 95% RH.
Results are shown for the same polymer substituted with nonamethyltriphenyl phosphonium cations (triangles), methyl pyrrolidinium cations (squares), methyl piperidenium cations (circles), or benzyltrimethylammonium, first-generation cations (diamonds).

I. Interaction of Peptides and Proteins with Abiotic Surfaces: Towards Water-Free Biologics
Investigator: Professor Zhan Chen, University of Michigan, MURI Award
Recipient: Imbed Biosciences, Inc.

The objective of this multidisciplinary research, led by Professor Chen at the University of Michigan, is to understand the properties that control biological-abiological interfaces and how to design systems for predicted biological structure and function. Professor Chen and his team have been focusing on the development of abiotic surfaces displaying hydromimetic functionalities that stabilize the native structure and function of biological molecules in the absence of bulk water. Towards this aim, it is critical to understand the water behavior at the abiotic surfaces for peptide and protein immobilization and the abiotic/biotic interfaces in air at different humidity levels. In FY16, co-PI Nick Abbott has studied the factors that influence the recruitment of water to surfaces that present a range of non-polar, polar and charged chemical functional groups of relevance to design of abiotic-biotic interfaces, including surfaces that present immobilized antimicrobial peptides. Quartz crystal microbalance with dissipation (QCM-D) studies revealed the central role that hydrogen bonding and charge interactions at surfaces play in recruitment of water. The results were shown to extend to the amino acid composition of immobilized peptides. Specifically, the number of charged residues within the peptide influence the recruitment of water to peptide decorated self-assembled monolayer surfaces (see FIGURE 14). Hybrid peptide, Cecropin A-Melittin, has five charged resides and recruits 1.3 water molecules per residue. Peptides with additional charged residues (Cecropin P1 (7); MSI-78 (8-9)) recruit 1.5-1.7 water molecules per residue. QCM-D studies also revealed that as peptide (Cecropin P1) surface coverage decreased from 0.3 peptide/nm^2 to 0.14 peptide/nm^2 to 0.1 peptide/nm^2, water adsorption increased from 1.5 to as much as 7 water molecules per residue before decreasing to 5 at the lowest peptide densities. Similar trends were observed for other peptides. These results suggest that a decrease in peptide surface coverage may decrease inter-peptide interactions on the surface, thus facilitating peptide-water interactions. In FY16, Professor Abbott transitioned this new understanding of factors that control recruitment of water to surfaces to Imbed Biosciences to enable the design and fabrication of new antimicrobial surfaces for advanced wound dressings.
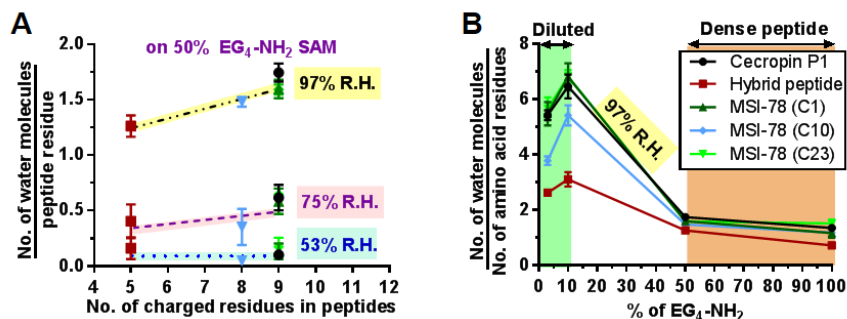
FIGURE 14

Recruitment of water to surfaces with immobilized antimicrobial peptides. (A) Number of water molecules per one residue of each of the five immobilized peptides at 97% RH versus the number of charged residues in peptides. (B) Number of water molecules per residue versus peptide surface coverage density (% of EG_4-NH_2 within SAMs).

J. Patterned Nanoporous Gold SERS Substrates

Investigator: Professor Sharon Weiss, Vanderbilt University, PECASE Award
Recipient: Molecular Diagnos-SERS

The objective of this research, led by Professor Weiss, was to systematically study the size-dependent infiltration, pre-concentration, and detection of small molecules into nanoscale porous silicon materials with tunable pore diameters between 10-100 nm. To successfully pattern porous materials with nanoscale resolution, Professor Weiss developed a one-step, direct patterning technique that does not require intermediate polymer processing or dry etching steps. Direct imprinting of porous substrates (DIPS) utilizes reusable stamps with micro- and nanoscale features that are applied directly to a porous material to selectively compress the porous network, resulting in the transfer of the stamp to the porous material with high fidelity, vertical resolution of 5 nm or less, and lateral resolution below 100 nm (see FIGURE 15). Using this process, both cost-effective and high performing porous silicon diffraction grating sensors and patterned nanoporous gold surface enhanced Raman scattering (SERS) substrates have been fabricated.

In FY16, Parks Technology licensed both the direct imprinting of porous substrates and nanoscale porous gold film SERS template inventions. Parks Technology has created a new company, Molecular Diagnos-SERS, to commercialize the patterned nanoporous gold SERS substrates.
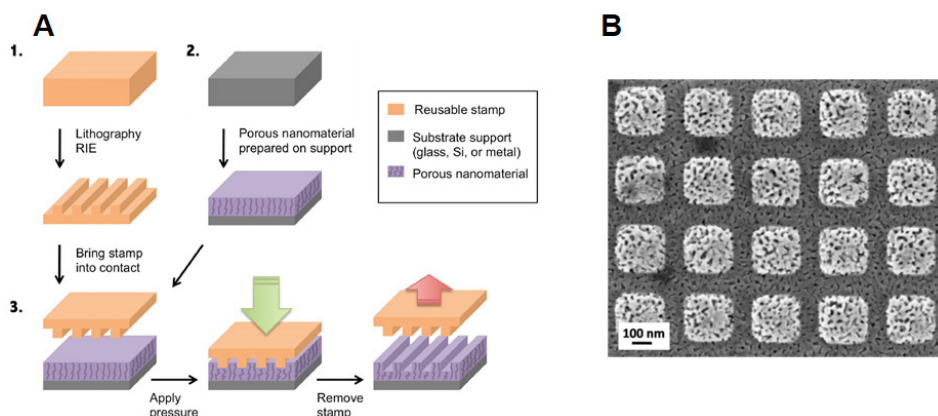

FIGURE 15

Direct imprinting of porous substrates (DIPS). (A) Illustration of DIPS technique; (B) SEM image of a representative surface morphology of a patterned nanoporous gold SERS template.

K. Foundational AISN Research Leads to Launch of Advanced Functional Fabrics of America
Investigators: Professors Yoel Fink, Steven Johnson, John Joannopoulos, MIT, Institute for Soldier Nanotechnolgies (UARC)
Recipient: Advanced Functional Fabrics of America (AFFOA)

AISN and MIT researchers, Professor Yoel Fink, Steven Johnson, and John Joannopoulos, have led ARO-funded research at the AISN since the Institute began. In FY16, U.S. Secretary of Defense Ash Carter announced the launch of the new Advanced Functional Fabrics of America (AFFOA) Institute, first proposed by Professor Fink based in part on ARL-sponsored multifunctional fiber research at the AISN, and Army collaborators at NSRDEC and ARL. AFFOA is a large scale private-public partnership that is a consortium of manufacturers, universities, and non-profits that is focused on MRL 4 to 7 advancements. Led by MIT with an ARDEC Program Manager, AFFOA's mission is to enable a manufacturing based revolution by transforming traditional fibers, yarns, and fabrics into highly sophisticated, integrated and networked devices and systems. The AFFOA Institute has the potential to create a whole new industry, based on the breakthroughs in fiber materials and manufacturing that have originated at the ARO sponsored AISN. Through multimaterial fiber device discoveries with radically new geometries and functions and by harnessing recently discovered phenomena such as fiber fluid instabilities, in-fiber phase transitions and novel crystallization mechanisms,, the novel technical textiles may advance multi-domain battle protection and situational awareness capabilities for the Soldier

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Metal/Lithium Fluoride/Lithium-Ion Electrolyte Interactions in Carbon Nanopores
Professor Gleb Yushin, Georgia Institute of Technology, Single Investigator Award

The objective of this research is to, for the first time, perform a systematic study to reveal the fundamental principles governing the metal/lithium fluoride/lithium-ion electrolyte interactions in a confined space of the carbon nanopores. The proposed study will reveal critical factors affecting the stability and electrochemical characteristics of nanoconfined metal fluorides and is expected to contribute to the development of stable, ultra-high energy density battery systems (see FIGURE 16).
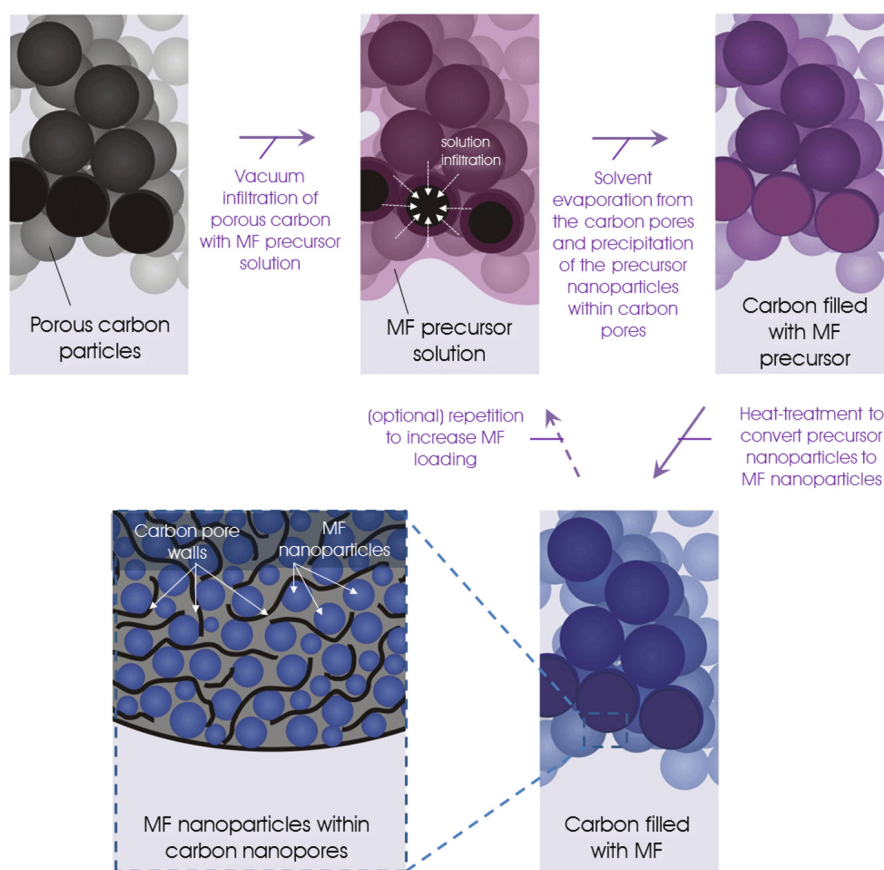
FIGURE 16
Schematic of the synthesis procedure of infiltration of metal fluorides (MF) into C nanopores.

This innovative research will change the way researchers design electrical energy storage materials and will contribute to the development of innovative and transformative energy storage technologies, critically needed for the DoD. At the most fundamental level, the proposed work will reveal the roles that the nanoscale curvature, surface chemistry, complex interfaces, electrolyte composition and molarity and various electrolyte reduction products may play in ion transport and electrochemistry in general and the way the porous nanocomposites can be designed to effectively regulate the nanoscale transport processes. It is anticipated that in FY17, the team

determine the impact of the pore size on the reversibility and rate of electrochemical reactions of nano-confined selected metal fluorides with Li ion electrolytes of various salt composition and concentrations. It is also expected that we will elucidate the influence of electrolyte and passivation layer structural and transport properties on the rate and reversibility of the conversion reaction of metal fluorides.

B. New Polymeric Materials Incorporating Heteromatic Phosphabenzene Units
Professor Kevin Noonan, Carnegie Melon University, Single Investigator Award

The objective of this research is to combine the concepts of sequence control with chain-growth polycondensation for semiconducting polymers. It is anticipated that in FY17, the Noonan laboratory will have prepared π-conjugated materials with narrow dispersities that consist of different monomer arrangements along the polymer backbone. These constructs are essential to explore how sequence changes along the backbone impact electronic structure as well as solid-state organization of the material (see FIGURE 17). Building from poly(3-hexylthiophene) as a benchmark, incorporation of different group 16 heterocycles (furan, selenophene and tellurophene) is under investigation. Additionally, systematic changes in the side chain of the polymer (ester, amide and cyano) is also being evaluated. To date, solid-state order (π-stacking and lamellar spacing) of periodic alkyl thiophene-selenophene copolymers has been shown to be strongly dependent on sequence. Remarkably, random copolymer analogues do not show the same dependence on content of the two monomers. Further studies are in process to better understand this observation, while also expanding to other monomers and side chains. These studies may provide insight into how perturbations along the polymer chain impact electronic transport in organic materials. These studies are likely to be relevant for future Army applications including chemical and biological sensing, as well as energy conversion.
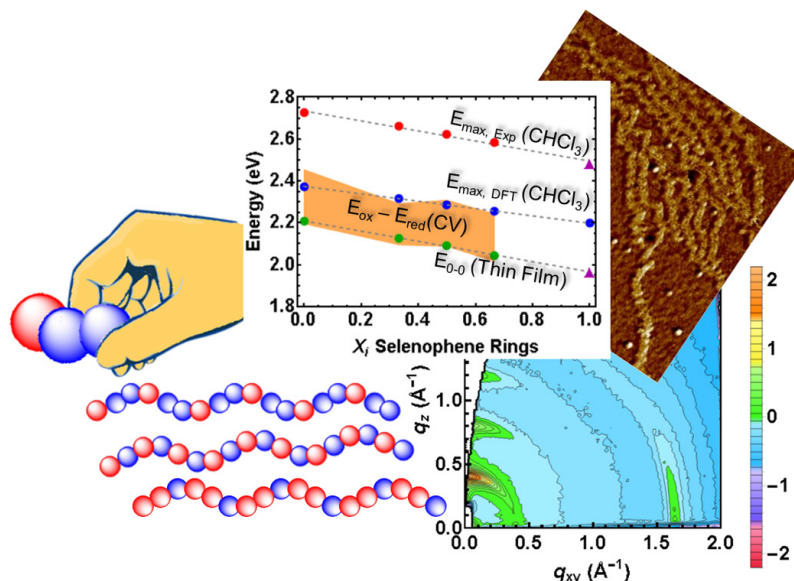

FIGURE 17

Impact of sequence on the electronic properties and solid-state organization of alkyl thiophene-selenophene copolymers.

C. Molecule-Surface Dynamics in Functionalized Mesoporous Silicon
Investigator: Professor Sharon Weiss, Vanderbilt University, Single Investigator Award

The objective of this research is to gain a fundamental understanding of the impact of porous silicon (PSi) functionalization chemistry and morphology on the surface interaction mechanisms involved in macroscopic diffusion and attachment of different chemical and biomolecular species in PSi films and membranes. This research will provide critical information of how molecular attributes such as polarity, size, and ionicity will affect transport through PSi films and membranes. Initial work in FY16 focused on understanding analyte transport and reaction in open- and closed-ended porous materials. A combination of theoretical and experimental studies indicated that a flow-through PSi membrane is most beneficial for facilitating analyte

transport under modest flow velocities (5-17 μL/min) and reduces the volume of solution required for analysis (see FIGURE 18). In addition, the flow-through scheme indicates improved mass transport for larger analytes (see FIGURE 19). Initial investigation of thermal carbonization of PSi as an alternate method of surface passivation compared to thermal oxidation was carried out.
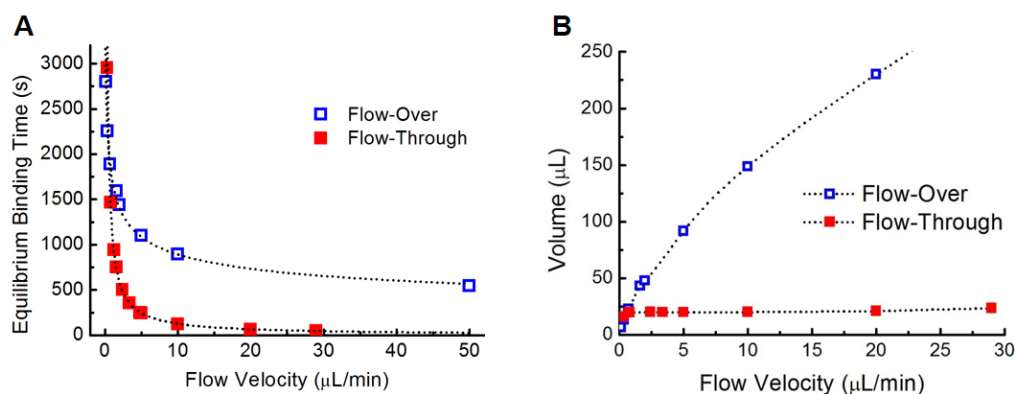

FIGURE 18

Comparison of transport kinetics in flow-through PSi membrane. The plots reveal the effect of flow velocity in (A) binding and (B) volume of consumed analyte.
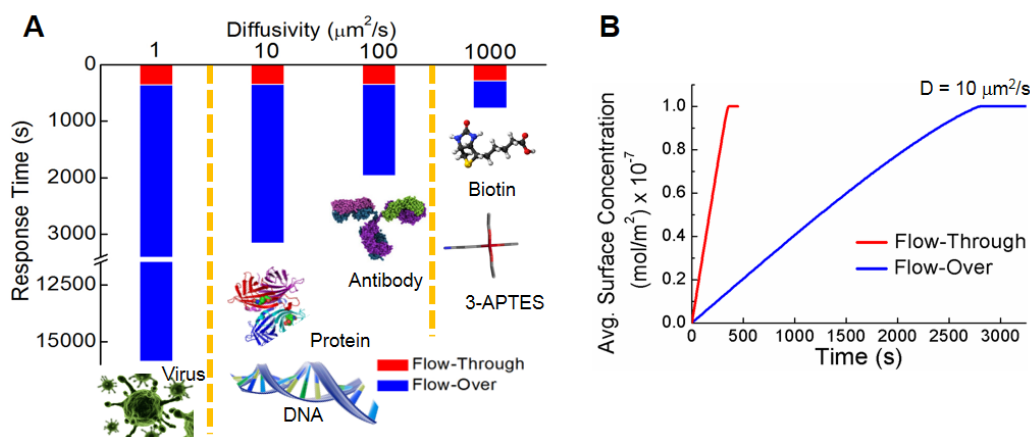
FIGURE 19

Flow-through scheme indicates improved mass transport for larger analytes. (A) Simulated sensor response time with various analytes; (B) simulated real-time response when D=10 $\mu m^2/s$.

In FY17, it is anticipated that the team will continue to refine the thermal carbonization techniques to achieve a graphene-like internal surface coverage in pores that sufficiently passivates the surface against chemical attack while maintaining the desired optical properties of the silicon films. In addition, the team will investigate different porous silicon morphologies and multilayer geometries that will provide a better understanding of mass transport and binding kinetics of small molecules in the pores. This effort will impact Army relevant areas in biosensing, filtration, and catalysis.

D. Effect of Strong Electron Correlation in the Description and Design of Efficient Energy Transfer Mechanisms
Professor David M. Mazziotti, University of Chicago, Single Investigator Award

The goal of this research is to significantly improve the ability of the variational two-electron reduced density matrix (2-RDM) method to treat strongly correlated excited states. It is anticipated that in FY17, the investigator will explore two complementary approaches: (i) the improvement of linear-response algorithms in which excited

states are extracted from the ground-state 2-RDM. Basic linear-response algorithms for the 2-RDM have been proposed and implemented by the investigator and others. However, there exist areas for improvement including the incorporation of better reconstruction of higher RDMs from lower RDMs as well as the generation of more consistent solutions of the generalized eigenvalue equation, and (ii) the development of direct excited-state algorithms in which the excited state 2-RDMs are directly computed by the variational 2-RDM method. The investigator will use a set of "orthogonality" conditions to remove the part of the 2-RDM's convex set that corresponds to the ground state. Minimization of the energy in the orthogonality-constrained set will directly generate the 2-RDM of the first excited state. Higher excited states will be obtained by including additional orthogonality constraints. Furthermore, the investigator will make improvements to the boundary-point algorithm for SDP, especially through the incorporation of stochastic sampling of projections onto the convex set to accelerate optimization with respect to the set in the context of an easily parallelizable algorithm. The investgator will also develop $O(r^4)$-scaling 2-RDM algorithms for treating very large molecules by exploiting sparse tensor techniques, including spatial locality and tensor factorizations, to represent both electron integrals and the 2-RDMs. This work will build upon a recent $O(r^4)$-scaling prototype 2-RDM algorithm. The investigator will develop a new 2-RDM based algorithm for molecular conductivity that can, in a practical way, treat conductance in strongly correlated molecules. There is currently no existing method that can do this. Finally, the investigator plans to extend the parametric 2-RDM method to excited states. In the parametric 2-RDM method the N-representability conditions are incorporated implicitly through the parameterization of the 2- RDM. The methods have a lower computational prefactor than traditional pair correlation methods such as coupled cluster with single and double excitations as well as the ability to capture some multi-reference correlation effects. The parametric 2-RDM method was developed with previous ARO support, and is available for download from the group's website. The method has been applied to diradical intermediates and transition states, such as the diradical isomers of olympicene and the transition state connecting *cis* and *trans* diazene, where it yields energies that are 10-15 kcal/mol lower than those from conventional single-reference wave function methods. Applications have also been made to studying the stability of oxywater and the relative energies of the cage and prism isomers of water hexamer. The investigator will develop a parametric 2-RDM method for excited states in which constraints are added to the energy functional to enforce a set orthogonality conditions, based on those in configuration interaction with single and double excitations. Excited states can also extracted from the ground-state 2-RDM by the linear-response algorithms to be further developed for 2-RDMs.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Robert Mantz
Division Chief (Acting)
Program Manager, Electrochemistry

Dr. James Parker
Program Manager, Molecular Structure and Dynamics

Dr. Dawanne Poree
Program Manager, Polymer Chemistry
Program Manager (Acting), Reactive Chemical Systems

Ms. Wendy Mills
Contract Support, Reactive Chemical Systems

B. Directorate Scientists and Technical Staff

Dr. Hugh De Long
Director (incoming), Physical Sciences Directorate

Dr. Douglas Kiserow
Director (outgoing), Physical Sciences Directorate

Dr. Peter Reynolds
Senior Scientist, Physical Sciences Directorate

Dr. J. Aura Gimm
Program Manager, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies

Dr. Kelby Kizer
Physical Scientist and Technical Assistant to the PSD Director

Mr. John McConville
Technology Transfer Officer, Institute for Soldier Nanotechnologies

C. Administrative Staff

Ms. Inez Kendall
Contract Support

Ms. Wanda Lawrence
Contract Support

CHAPTER 4: COMPUTING SCIENCES DIVISION

I.   OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2016* is to provide information on the programs and basic research supported by ARO in fiscal year 2016 (FY16), and ARO's mission to create basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Computing Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and transitions facilitated by this Division in FY16.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of the ARO Computing Sciences Division is to build the fundamental principles and techniques governing computational methods, models, and architectures to establish the foundation for revolutionary advances in intelligent, trusted, and resilient computing that provide increased performance and computational capability to enhance warfighter situational awareness, decision making, command and control, and weapons systems performance. The Division supports basic research in new computing architectures and models for intelligent and trusted computing in data fusion and extraction techniques for efficient information processing, to create new capabilities in social informatics, and in resilient computing systems for mission assurance. The results of these efforts will stimulate future studies and help keep the U.S. at the forefront of computing sciences research.

2. Potential Applications. This program identifies and addresses the Army's critical basic research problems in the computing sciences where progress has been inhibited by a lack of novel concepts or fundamental knowledge. Computing science is pervasive in nearly all Army systems, particularly Command, Control, Communications, Computing, Intelligence, Surveillance, and Reconnaissance (C4ISR) systems. The number of information sources on the battlefield will grow rapidly; computing and information science research must provide capabilities to process this in real-time and ensure that Soldiers and commanders do not experience information overload that could adversely affect their ability to make decisions. Also, in spite of the increased complexity of future battlefield information systems, dependence on them will only increase, therefore they must be extremely reliable and secure. Research in this program has application to a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the Army's Future operational goals. For this reason, computing science is a key technology underpinning future Army operations.

3. Coordination with Other Divisions and Agencies. The Computing Sciences Division supports ARL's Information Sciences Campaign in the areas of information understanding, information fusion, and computational intelligence. Collaborative efforts aim at discovering scientific principles and creating innovative frameworks and analytical approaches for the representation, dimensionality reduction, information content extraction, and integration of multimodal data that will revolutionize information processing to convert data into actionable intelligence to support Army information processing. A joint workshop was organized by the division and the ARL Cyber Security Research Consortium to explore new research opportunities in moving target cyber defense. The Computing Sciences Division has worked with ARL's Computational and Information Sciences Directorate (CISD) to develop two new Small Business Technology Transfer (STTR) projects that will enhance computational capability through novel computing system architectural design. Division staff have engaged the ARL Human Sciences Campaign and the Sciences-for-Lethality and Protection Campaign to create a new computer simulation capability for acoustic modeling for human studies and for radio frequency (RF) propagation in urban environments.

The Division's research investment strategy is coordinated with partner disciplines and computer scientists at ARO, other directorates within ARL, other Army agencies, and related programs in other DoD and Federal organizations. The Division's research portfolio is supported by Army basic research Core funding with substantial additional resources from the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)], including the Multidisciplinary University Research Initiative Program (MURI), and from other agencies, such as the Defense Advanced Research Projects Agency (DARPA).

To effectively meet Division objectives and to maximize the impact of potential discoveries for the Army and the nation, the Computing Sciences Division frequently coordinates and leverages efforts with Army scientists and engineers and with researchers in other DoD agencies. In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the ARO Life Sciences Division include promoting research to investigate effective human-computer communication mechanisms and developing new metrics and benchmarks for social media analysis. The Division also coordinates efforts with the Network Sciences Division to explore new techniques for robust and resilient mobile ad hoc networks, to establish adversarial models for effective cyber defense, and to investigate fundamental principles for trusted social computing. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas. Each of the Program Areas within the Division balances opportunity-driven research with high risk, high-payoff scientific exploration and needs-driven efforts that look for scientific solutions to the near-term needs of the warfighter.

B. Program Areas

The Computing Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY16, the Division managed research within these four Program Areas: (i) Information Processing and Fusion, (ii) Computational Architectures and Visualization, (iii) Information and Software Assurance, and (iv) Social Informatics. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Information Processing and Fusion. The goal of this Program Area is to understand the fundamental principles and to establish innovative theories for data processing, information extraction, and information integration toward real-time situational awareness and advanced targeting. There are three thrusts for this program area: (i) foundations of image and multimodal data analysis, (ii) data and information fusion, and (iii) active and collaborative sensing. With the ubiquitous availability of data acquisition capabilities in future military operations, effective data and information processing is of increasingly critical importance to defense missions. This program emphasizes mathematical theories, methodologies and algorithms for image understanding, video analysis, and data/information fusion. This research supports the development of novel representations of multimodal data to enable the understanding of multimodal sensor data and contextual information. Also supported is research on detection of events, actions, and activities to extract activity-based intelligence, especially when the events are rare and no extensive training data is available. Potential applications include detection of improvised explosive devices and persistent surveillance.

The increased capability of electronic systems and the proliferation of sensors are generating rapidly increasing quantities of data and information to the point that system operators and commanders are overwhelmed with data and saturated with information. An area of increasing importance is data and information integration or fusion, especially fusion of data from disparate sensors and contextual information. Research activities address several basic issues of data fusion, including information content characterization of sensor data, performance modeling, and the value of information.

2. Computational Architectures and Visualization. The two main Thrusts of this Program Area are Computational Architectures (CA) and Visualization (V). The goal of the CA Thrust is to discover new effective architectures, computational methods, and software tools for future computing systems with special emphasis on the effect that the technological shift to heterogeneous, multi-core processors will have on newly-developed systems. The goal of the V Thrust is to make very large simulations and the visualization of massive data sets

more computationally efficient and more interactive for the user. An overarching theme for both Thrusts is the efficient managing and processing of massive data sets. This is due to the fact that the Army's ability to generate data of all types from the battlefield to the laboratory far outpaces the Army's ability to efficiently manage, process, and visualize such massive amounts of information. The CA Thrust attempts to address this issue by investigating innovative architectural designs of both hardware and software components and their interfaces. The V Thrust addresses the issue by investigating innovative algorithms to render massive data sets and/or massive geometric models and to perform large scale simulations of importance to the Army.

The long-term payoffs of the CA Thrust for the Army include new computer modeling and design concepts (or paradigms) as well as software libraries that take advantage of these new multi-core processors and that are scalable (usable on large-scale complex problems and able to handle massive amounts of data) and accurate (precise enough to predict and detect phenomena of interest) for both the laboratory and the battlefield. A payoff associated with the V Thrust is the development of more efficient, interactive, and physically realistic battlefield, training, and scientific simulations.

3. Information and Software Assurance. The goal of this Program Area is to understand the fundamental principles of robust and resilient cyber information systems that can enable the corresponding functions to be sustained under adversarial conditions. The studies guided by this program will enable and lead to the design and establishment of trustworthy computing and communication, regardless of threat conditions. The ARO program on Information Assurance currently has two major Thrust areas: (i) Highly Assured Tactical Information and (ii) Resilient and Robust Information Infrastructure. The goal of the Highly Assured Tactical Information Thrust is to gain new scientific understandings for trustworthy tactical communications and for establishing fundamental principles and to ensure their trustworthiness. The Resilient and Robust Information Infrastructure Thrust promotes research on cyber situation awareness theories and frameworks that combines intrusion prevention, detection, response, and recovery to establish fundamental scientific principles for building mission-sustaining information systems (e.g., software/hardware, computing/communication systems).

Within these research areas, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. Research in the Resilient and Robust Information Infrastructure Thrust is focused on exploring and establishing resilient computing and survivability principles, and understanding system trade-offs such as performance, resiliency, and, survivability. The Highly Assured Tactical Information Thrust may lead to the development of novel situation awareness theories and techniques that help defenders obtain an accurate view of the available cyber-assets, to automatically assess the damage of attacks, possible next moves, and impact on cyber missions, and to model the behavior of adversaries to predict the threat of future attacks on the success of a mission. The warfighters must have unprecedented situational awareness (including enemy and friendly awareness) at all times. Information assurance must address the delivery of authentic, accurate, secure, reliable, timely information, regardless of threat conditions, over heterogeneous networks consisting of both tactical (mobile, wireless) and fixed (wired) communication infrastructures.

4. Intelligent Systems. The goal of this Program Area is to establish the scientific foundation of next generation intelligent systems and create cutting-edge capabilities in machine learning that can greatly enhance the Army's capabilities in mobility, agility, lethality, and survivability. There are two main research thrust areas: (i) Advanced Learning and (ii) Intelligent Systems.

The Advanced Learning thrust focuses on establishing the theoretical foundation of machine learning. New learning approaches will need to be addressed for both dimensionality challenges and temporal characterization of "big data," which may evolve continuously. In addition, new techniques must address robustness where the learning system will be able to deal with incorrect input due to noise and observation errors, and potentially malicious input that aims to disrupt learning. Adaptation in learning is another major challenge. It is conceivable that due to complexity, non-steady behaviors, fast changing context and environment, it may not ever be possible to fully capture a dynamic changing world, especially under the condition of incomplete information and with information uncertainties. It is critical to develop an advanced system that can continuously learn, update its knowledge base accordingly, and dynamically adapt its reasoning, decisions, and actions.

The Intelligent Systems thrust focuses on creating autonomous entities with advanced cognitive capabilities that can successfully integrate advanced learning, knowledge representation and organization, cognitive reasoning, adaptation, and autonomous action. Quite often intelligence systems are engaged in sensing, perception, reasoning and understanding, learning, collaboration, and take actions in an autonomous way. For these systems, sensing and vision processing play a critical role in learning, perception, and establish situation awareness for decision making and for intelligent actions such as navigation, while language processing and communication help build coordination, collaboration, and contribute to a shared knowledge base, planning, and team decision making. A common trait of intelligent systems lies in their capability to process information along with suitable context and environment to make the best decisions and to take appropriate actions. An ideal intelligence system should have a strong cognitive capability that enables itself to deal with environmental changes, to carry out new tasks, and to cope with unknown situations.

C. Research Investment

The total funds managed by the ARO Computing Sciences Division for FY16 were $19.4 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $5.3 million and $1.2 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $5.4 million to projects managed by the Division. The Division also managed $5.6 million of Defense Advanced Research Projects Agency (DARPA) programs. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.7 million for contracts. In addition, $2.1 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.9 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY16 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY16 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY16, the Division awarded 18 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Gail-Joon Ahn, Arizona State University; *Dissecting Social Dynamics and Malware Attributions for Mitigating Network-centric Attacks*
- Professor Reza Azarderakhsh, Rochester Institute of Technology; *Emerging Side-channel Resistant and Resource-friendly Elliptic Curve Algorithms and Architectures*
- Professor William Enck, North Carolina State University; *Correct Enforcement of Access Control Policy in Modern Operating Systems*
- Professor Timothy Havens, Michigan Technological University; *Multisensor Analysis and Algorithm Development for Detection and Classification of Buried and Obscured Targets*
- Professor Thomas Huang, University of Illinois at Urbana - Champaign; *Very Low-Resolution Face Recognition In The Wild*
- Professor Yier Jin, University of Central Florida; *Bridging the Hardware-Software Gap: A Proof-Carrying Approach for Computer Systems Trust Evaluation*
- Professor Ari Juels, Cornell University; *Toward Principled Foundations for Honey Objects in Information Security*
- Professor Ming Lin, University of North Carolina - Chapel Hill; *Efficient Computational Models for Simulating Large-Scale, Heterogeneous Crowds*
- Professor Vishal Patel, Rutgers University - New Brunswick; *Adaptive Sparse and Low-Rank Models for Real-World Visual Recognition*
- Professor Radha Poovendran, University of Washington; *Multi-Layer Adaptive and Proactive Strategic Cyber Defense*
- Professor Balakrishnan Prabhakaran, University of Texas at Dallas; *Robust 3D Surveillance*
- Professor Aswin Sankaranarayanan, Carnegie Mellon University; *Scalable Inference on High-Dimensional Data via Task- and Domain-Specific Embeddings*

- Professor William Scherlis, Carnegie Mellon University; *Global Mapping of Cyber Security Threats: Actual and Perceived*
- Professor Jinyuan Sun, University of Tennessee at Knoxville; *Security Through Invisibility for Dynamically Changing Wireless Sensor Networks*
- Professor Gene Tsudik, University of California - Irvine; *Remote Attestation of Critical Infrastructure Components*
- Professor Xiaofeng Wang, Indiana University at Bloomington; *How to Compose Security Protection for Third-Party Applications*
- Professor Ying Wu, Northwestern University - Evanston; *Handling Adverse Visual Conditions for Target Tracking and Recognition*
- Professor Ning Xi, The University of Hong Kong; *Compressive Feedback for Featureless Video-based Tracking Control*

2. Short Term Innovative Research (STIR) Program. In FY16, the Division awarded 10 new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Leonardo Bobadilla, Florida International University; *Gathering and Processing Sensor Data with Unmanned Relay Vehicles using Line-of-Sight Communication*
- Professor Vasiliki Ikonomidou, George Mason University; *Change Point Detection for Video-Based Stressor Identification*
- Professor Sundararaj Iyengar, Florida International University; *Scientific Exploration of Cyber-Driven Dynamic, Distributed Big Data Forensics Systems*
- Professor Hamid Krim, North Carolina State University; *Neuron-based Measurements for Brain Functionality Understanding*
- Professor Yue Lu, Harvard University; *Analyzing the Large System Limit of Stochastic Proximal Gradient Methods for Online Estimation*
- Professor Nasser Nasrabadi, West Virginia University; *Task-Driven Coupled Dictionary Design for Heterogeneous Sensory Data*
- Professor Gang Qu, University of Maryland - College Park; *Building Robust and Practical Physically Unclonable Functions with Configurable Ring Oscillators*
- Professor Carlo Tomasi, Duke University; *Multiscale Path Metrics for the Analysis of Discrete Geometric Structures*
- Professor Dong Wang, University of Notre Dame; *Quality-of-Information-Aware Data Collection and Analysis for Active and Collaborative Sensing*
- Professor Yue Wang, Clemson University; *Trust-based Optimal Guidance and Navigation for Multiple Manned-Unmanned Vehicles*

3. Young Investigator Program (YIP). In FY16, the Division awarded one new YIP project to drive fundamental research in an area relevant to the current and future Army. The following PI and corresponding organization was a recipient of the new-start YIP award.

- Professor Domenic Forte, University of Florida - Gainesville; *Human-to-Device: A Novel Anti-Tampering Mechanism Driven by Cardiovascular Biometric and Obfuscation*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY16 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *US-Europe Workshop on Cryptography and Hardware Security for the Internet of Things*; College Park, MD; 8-9 October, 2015
- *Trustworthy Human-Centric Social Networking: Challenges and Research Directions*; Phoenix, AZ; 12-13 May 2016
- *Institute of Electrical and Electronics Engineers (IEEE) Symposium on Security and Privacy*; San Jose, CA; 23-25 May 2016

- *2016 Image Science Gordon Research Conference*; Easton, MA; June 5-10, 2016
- *The Optical Society (OSA) Imaging Systems and Applications Conference*; Heidelberg, Germany; 25-28 July 2016
- *OSA Computational Optical Sensing and Imaging Conference*; Heidelberg, Germany; 25-28 July 2016
- *Workshop on Multimodal Data Analysis for Human Activity Detection and Understanding*; Marina del Rey, CA; 23-24 August 2016
- *23rd IEEE International Conference on Image Processing*; Phoenix, AZ; 25-28 September 2016

5. Special Programs. In FY16, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded four new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Computing Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Value-centered Information Theory. This MURI began in FY11 and was awarded to a team led by Professor Alfred Hero III at the University of Michigan. The objective of this MURI is to lay the foundation for a new information theory that applies to general controlled information gathering and inference systems and accounts for the value of information. The theory will be built on a foundation of non-commutative information theory, free probability theory, differential geometric representations of information, and the theory of surrogate information measures. This theory will improve the scientific understanding of the fundamental limits of performance and create better algorithms for extracting and exploiting information in distributed sensor systems.

This research focuses on multiple-modality multiple-sensor fusion problems that use consensus fusion, contextual graphical models, gossip algorithms, and likelihood maps to aggregate information for tracking, surveillance, and other tasks. Topics of interest include resource management in adversarial environments, mobile sensors, and multistage mission planning. Emphasis is placed on creating a powerful theory of actionable information that accounts for value of information and the economic costs of deploying or maneuvering sensors to achieve a particular mission objective. The research comprises three inter-related research themes that collectively address the most critical research challenges in distributed sensing. These thrusts are: (i) information-driven structure learning and representation, (ii) distributed information fusion, and (iii) active information exploitation for resource management. An end-to-end framework will be created that will result in better raw sensor data acquisition and processing, more accurate multi-target tracking, and improved fusion.

3. Adversarial and Uncertain Reasoning for Adaptive Cyber Defense: Building the Scientific Foundation. This MURI began in FY13 and was awarded to a team led by Professor Sushil Jajodia of George Mason University. Adaptive defense mechanisms are essential to protect our nation's critical infrastructure (computing, communication, and control) from sophisticated adversaries who may stealthily observe defense systems and dynamically adapt their attack strategies. This research aims to create a unified scientific foundation to enable the design of adaptive defense mechanisms that will maximize the protection of cyber infrastructure while minimizing the capabilities of adversaries.

The research will leverage recent advances in security modeling, network science, game theory, control theory, software system and network protocol security to create the scientific foundation, which may include general models for defense mechanisms and the systems they protect as well as irrational and rational adversaries. This research will develop a new class of technologies called Adaptive Cyber Defense (ACD) that will force adversaries to continually re-assess, re-engineer and re-launch their cyber attacks. ACD presents adversaries

with optimized dynamically-changing attack surfaces and system configurations, thereby significantly increasing the attacker's workloads and decreasing their probabilities of success.

4. Noncommutativity in Interdependent Multimodal Data Analysis. This MURI began in FY16 and was awarded to a team led by Professor Negar Kiyavash at the University of Illinois at Urbana-Champaign. The goal of this research is to establish a new comprehensive information theory for data analysis in noncommutative information structures intrinsic to hierarchical representations, distributed sensing, and adaptive online processing. Methods will be developed based on a novel theory in conjunction with the latest theories of information, random matrices, free probability, optimal transport, and statistical machine learning. They will be applied to the technical domains of causal inference, adaptive learning, computer vision, and heterogeneous sensor networks, and will be validated on real-data test beds including: (i) human action and collective behavior recognition, and (ii) crowd-sourcing in a network of brain-machine interfaces. The framework will provide answers to questions such as: What are the fundamental performance limits for noncommutative information collection and processing systems? What is the effect of side information on noncommutative information structures? How can low complexity proxies for performance be defined that approximate or bound noncommutative performance limits? How can noncommutativity of adaptive measurements be exploited to improve fusion, processing, and planning for distributed sensing systems? When do sequential or partially ordered designs offer significant performance gains relative to randomized designs like compressive sensing?

The approaches for extracting knowledge from complex irreversible partially ordered information structures include but are not limited to introduction of information divergence measures over noncommutative algebras, noncommutative relative entropy measures, and estimation techniques for such measures for high-dimensional data. Accounting for noncommutative structures will result in fundamentally new ways of fusing ordered, directed, or hierarchical organized information in order to support timely decisions at the appropriate level of granularity. Humans learn actively and adaptively, and their judgments about the likelihood of events and dependencies among variables are strongly influenced by the perception of cause and effect, whereas man-made systems only employ correlation-type symmetric measures of dependencies. Research will lead to the development of a theory of decentralized information sharing, causal inference, and active learning inspired by human decision making. Establishment of such a theory for sensing and data processing and application of it to grand challenges in computer vision and brain-computer interfaces will provide new capabilities, including improved time-sensitive, dynamic, multi-source information processing, actuation, and performance prediction guarantees.

5. Closed-Loop Multisensory Brain-Computer Interface for Enhanced Decision Accuracy. This MURI began in FY16 and was awarded to a team led by Professor Maryam Shanechi at the University of Southern California. The goal of this research is to create new methodologies for modeling multimodal neural activity underlying multisensory processing and decision making, and to use those methodologies to design closed-loop adaptive algorithms for optimized exploitation of multisensory data for brain-computer communication.

This research effort will contribute to the development of a new closed-loop brain-computer interface (BCI) framework for enhancing decision accuracy. The framework will collect multimodal neural, physiological, and behavioral data, decode mental states such as attention orientation and situational awareness, and use the decoded states as feedback to adaptively change the multisensory cues provided to the subject, thus closing the loop. To realize such a framework, the effort will make fundamental advances on four fronts, constituting four research thrusts: (1) modeling multisensory integration, attention, and decision making, and the associated neural mechanisms; (2) machine-learning algorithms for high-dimensional multimodal data fusion; (3) adaptive tracking of the neural and behavioral models during online operation of the BCI; and (4) adaptive BCI control of multisensory cues for optimized performance. Complementary experiments with rodents, monkeys, and humans will be conducted to collect multimodal data to study and model multisensory integration, attention, and decision making, and to prototype a BCI for enhanced decision accuracy. The modeling efforts will span Bayesian inference, stochastic control, adaptive signal processing, and machine learning to develop: (1) novel Bayesian and control-theoretic models of the brain mechanisms; (2) new stochastic models of multimodal data and adaptive inference algorithms for this data; and (3) novel adaptive stochastic controllers of multisensory cues based on the feedback of users' cognitive state.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY16.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES. In FY16, the Division managed three new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase I contracts and one Phase II contract. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY16 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY16, the Division managed two new ARO (Core) HBCU/MI projects and four new REP awards, in addition to active projects continuing from prior years. Refer to CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY16.

G. Defense University Research Instrumentation Program (DURIP)

As described in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY16, the Division managed nine new DURIP projects, totaling $1.8 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. Joint NSA/ARL-ARO Advanced Computing Initiative

The Advanced Computing Initiative (ACI) is an ongoing NSA/ARL-ARO joint venture on energy efficient computing. Specifically, energy efficiency is now a primary constraint in designing new supercomputers. In order to provide robust performance, future systems will need to be able to dynamically trade off energy efficiency, performance, and reliability. Initiated in FY13, the ACI program's objective is to support research for enabling these tradeoffs and will run for four years at approximately $4 million/year. ARO is responsible for the program management and contracting duties. The ACI program has a close relationship to ARL's High Performance Computing efforts and they offer potential cost savings and reliability benefits for the Army. The costs associated with consuming megawatts of electricity both directly and for the elaborate cooling systems to deal with the excessive heat supercomputers generate are becoming excessive. More important is the machine's reliability as more power to the system means more heat to the components, significantly increasing failure rates. Developing hardware and software infrastructure to increase performance while ignoring the effects on power consumption and reliability will not be feasible in the future. Seven grants have been awarded under the ACI program to teams composed of members from academia, industry and the national laboratories.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Computing Sciences Division.

A. Modeling Interrelations for Understanding and Predicting Complex Human Behavior
Professor Silvio Savarese, Stanford University, MURI Award

The goal of this research is to establish new comprehensive information theory for data analysis in noncommutative information structures intrinsic to hierarchical representations, distributed sensing, and adaptive online processing. Non-commutativity is exploited in problems of computer vision including object pose estimation and recognition, human action and interaction analysis, and collective behavior tracking. Human action recognition is an extremely important research area in computer vision, and has grown dramatically in the last decade. This recognition problem involves fusion of visual information over multiple time and spatial scales extracted from videos and video databases.

In FY16, Professor Savarese and his team established and applied a new class of tools for addressing non-commutative action sequence recognition based on ordinal 3D+t spatiotemporal segment models, non-commutative information theoretic discriminants, and variational inference, particularly deep learning on spatiotemporal graphs. Deep Recurrent Neural Network architectures, though remarkably capable at modeling causal sequences, lack an intuitive high-level spatiotemporal structure. That is why many problems in computer vision inherently have an underlying high-level structure and can benefit from it. Spatiotemporal graphs are a flexible tool for imposing such high-level intuitions in the formulation of real world problems. The research team developed an approach for combining the power of high-level spatiotemporal graphs and effective non-commutative sequence learning using Recurrent Neural Networks (RNNs). A scalable method was created for casting an arbitrary spatiotemporal graph as a rich RNN mixture that is feedforward, fully differentiable, and jointly trainable (see FIGURE 1). This approach, called Structural-RNN, is generic and principled as it can be used for transforming any spatiotemporal graph through employing a certain set of well-defined steps. The evaluations of this approach on a diverse set of problems, ranging from modeling human motion to object interactions, show improvement over the state-of-the-art with a large margin, as much as 44%. This work received the Best Student Paper Award at the 2016 Institute of Electrical and Electronics Engineers (IEEE) Conference on Computer Vision and Pattern Recognition.
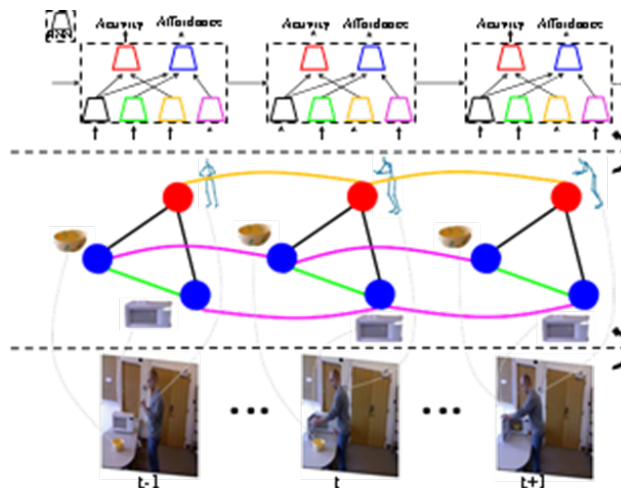

FIGURE 1

Illustration of S-RNN over spatiotemporal graph. *(Bottom)* An example activity (human microwaving food). Modeling such problems requires both spatial and temporal reasoning. *(Middle)* Spatio-temporal graph capturing spatial and temporal interactions between the human and the objects. *(Top)* Schematic representation of Structural-RNN architecture automatically derived from the spatiotemporal graph

B. A Comprehensive Model for Adversary and the Defender Interaction
Professor V. Subrahmanian, University of Maryland - College Park, Single Investigator Award

The goal of this research is to establish a rigorous scientific framework that can be used to guide the development of effective deception and disclosure strategies in a cyber security context to defeat cyber attacks. A major problem in understanding both the adversary and the defender is the enormous attack surface that is present in information systems. In order to understand how adversaries operate, it is important to understand the environment in which they operate, namely the enterprise network of the system being protected. Every piece of software and hardware, every protocol that is used, affords some opportunities for the attacker.

In FY16 Prof. Subrahmanian successfully created an attacker-defender game model that leads to the ability to reason about such a complex space with sophisticated probabilistic modeling of the attacker, the environment, and the defender that helps predict how an attacker will respond to the defense actions, and used those predictions to better defend cyber systems (see FIGURE 2). Based on such a model of the adversary, the team developed a mechanism by which the network can be modified by the defender so as to induce deception by placing honey nodes and apparent vulnerabilities into the network to distract and mislead the adversary. The team created the first algorithms to build a game-theoretic model that can be used to guide system patching and deactivations in order to minimize both the expected damage and the probability of the attacker succeeding. The team used the model to experiment with various attacker and defenders settings. The prototype implementation identified the best defense strategies given different attacks predications.
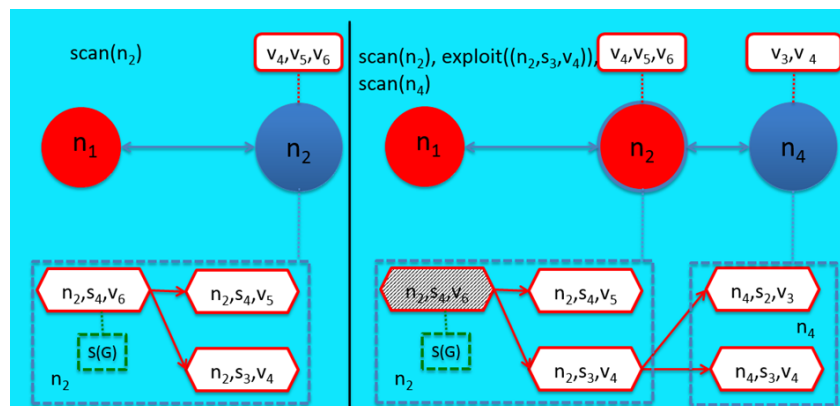

FIGURE 2

Example of system vulnerabilities dependency graph. The graph shows potential paths adversaries can take to intrude enterprise systems.

C. Fundamentals of Human Re-identification in Videos of Crowds
Professor Mubarak Shah, University of Central Florida, Single Investigator Award

The objective of this research is to create methods for automatic re-identification in dense crowds that allows successful monitoring and analysis of crowded events. Re-identification in crowded scenes is a challenging problem due to the large number of people and frequent occlusions, coupled with changes in their appearance due to different properties and exposure of cameras.

In FY16, Professor Shah and his team worked towards creating a new framework for re-identification of a large number of humans across multiple non-overlapping cameras, crucial both in the battlefield as well as post-event analysis in surveillance networks. They explicitly modeled multiple personal, social, and environmental constraints on human motion across cameras in crowded scenes. The personal constraints include appearance and preferred speed of each individual, while the social influences are modeled by grouping and collision avoidance. The environmental constraints model the transition probabilities between gates (entrances/exits) in different cameras. These constraints were incorporated into an energy minimization framework for solving human re-identification. Experimental results demonstrated the applicability of these cues for re-identification, achieving a significant boost in performance and accuracy over existing appearance-based approaches. The comparison of different constraints using Cumulative Matching Characteristics was performed. The introduction of linear constraint of preferred speed gives an improvement of 19%. Quadratic constraints of grouping were

considered to improve performance, with social grouping contributing about 6% improvement while spatial grouping added another 6% improvement. Finally, collision avoidance was employed, which gives the maximum Area Under Curve (AUC) of 96.15%.

D. In Situ Visualization of High-Order Methods
Professors Robert M. Kirby, University of Utah, and Robert Haimes, Massachusetts Institute of Technology, Single Investigator Award

The objective of this research is to create the theory and framework for a scalable in situ (while the calculations are proceeding) visualization system for any PDE-based solver (independent of whether it is high-order or not), that performs in situ visualization of higher-order results in a pixel-exact manner. Many current scientific visualization techniques applied to higher-order solutions are inadequate when used for knowledge extraction and assistance in reducing the error budget. This is because they transform high-order data to low-order representations for visualization purposes – a process which in and of itself adds "visualization error" to the error budget. The scientist is currently burdened with determining whether or not an anomaly found in an image generated by a visualization technique is from the modeling and discretization assumptions made as part of the simulation or as part of the visualization technique itself. In most cases that burden is high. In addition, many of the physical problems of interest are not steady-state, leading to simulations that must run for a long time (days, weeks, and in some cases months). The transient nature of these simulations complicates the data handling (post processing requires the time history) and renders single snap-shots of the solution, insufficient to understand the time-varying nature of the physics. There is now a growing acceptance in the simulation and visualization communities that in situ processing is the most effective and least intrusive way to understand the results from transient simulations. The goals of this effort are: (1) to generate "high-order Finite Element Method (FEM)" appropriate dimensionality reduction feature extraction methods which can be accomplished as part of an in situ data processing pipeline, and (2) specify the regions of interest in an in situ fashion within a simulation field based upon the visualization objective, extract and transmit relevant high-order FEM modal information to the visualization system, and then reconstruct the visualization features of interest (e.g., isosurfaces) in a pixel-exact fashion.

In FY16, this team of researchers created algorithms and software for extracting vortex core lines (i.e. areas of high swirl) from high-order (high-accuracy and high-fidelity) fluid flow simulations in situ (see FIGURE 3). This is extremely important to the Army as it allows Army engineers to understand the impact of various mission requirements in aeroacoustics and fluid-structure scenarios as found with Army rotorcraft. Vortex cores generated by rotor blade tips impinge on the body of the vehicle which creates the acoustic signature and directly impacts the fatigue of the craft's structures. Accurately simulating the location, trajectory, and intensity of vortex cores helps engineers produce better designs. These researchers are the first to be able to accurately extract such high-order derived vortex tube information in situ. This research will have a significant impact at the U.S. Army Aviation and Missile Research, Development, and Engineering Center (AMRDEC), who has had input on the formation of the research by allowing AMRDEC engineers to fully exploit the simulation results their teams generate for various mission scenarios.
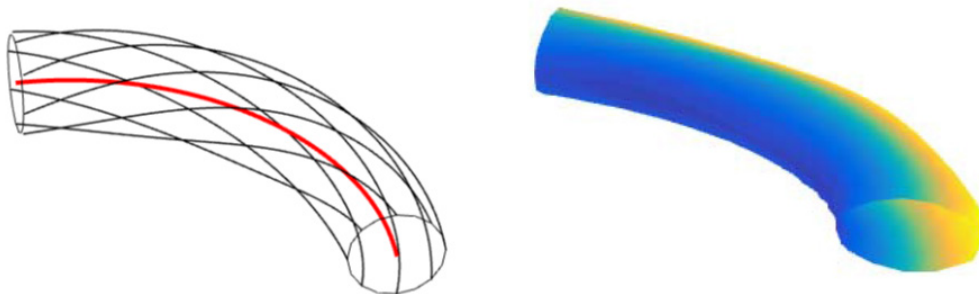

FIGURE 3

In situ visualization of high-order methods. (*left*) *V*ortex tube denoted by a core line and streamlines that give its surface envelope; (*right*) a vortex tube isosurface showing the magnitude of torsion. These extracted tubes are for synthetic high-order data generated by Utah's in situ methodology.

E. Improved Vulnerability Detection for Cybersecurity in Army Computing Systems
Professor John Cavazos, University of Delaware, Single Investigator Award

The goal of this research is to develop methods that will automatically allow for the rapid detection of software vulnerabilities in computer code without the need for access to the source code of the application nor human intervention. With the rapid growth of malware worldwide (see FIGURE 4) and the danger such malicious code presents to any and all computer systems, including the Army's, it has become critical that vulnerabilities in software be identified quickly, efficiently, and effectively. However, state-of-the-art detection techniques require access to the source code and are performed manually, taking from days to weeks to accomplish which is both slow and costly. Also, source code is not always available for analysis, e.g., the code may be closed-source or contain proprietary information.

In FY16, this team of researchers created a software framework for vulnerability detection in computer machine code executables (e.g. Applications or Apps) that unlike current methods, does not require access to the developer written source code (a program written in human-readable computer language). This is extremely important to the Army as source code is not always available for analysis. This vulnerability detection framework is modular and pipelined to allow scalable analysis on distributed systems. This research will have a significant impact at the CERDEC, who co-funds this effort, by allowing CERDEC engineers to very quickly and accurately analyze many millions of lines of assembly code from binaries, significantly reducing the time and effort necessary to assure the safety and reliability of Army computing systems.
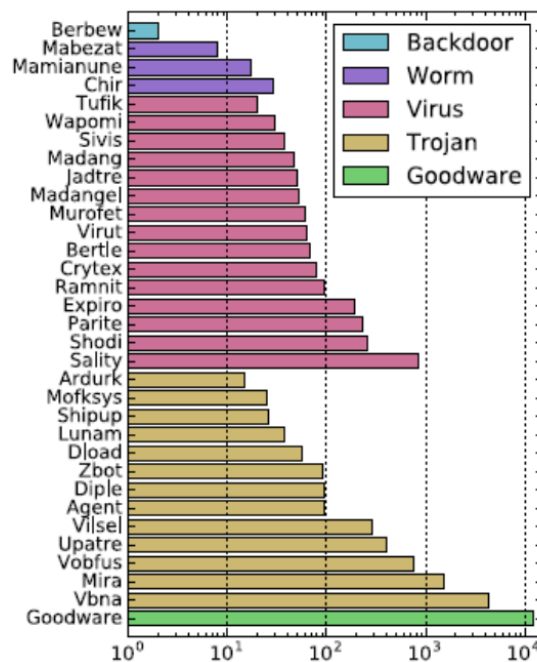

FIGURE 4

Rapid growth of malware. Bar graph depicting the magnitude of the number of instances (x-axis) that different types of malware (y-axis) has appeared on computer systems worldwide.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Fusion of Statistically Dependent Heterogeneous Information Sources
Investigator: Professor Pramod K. Varshney, Syracuse University, Single Investigator Award
Recipient: ARL Sensors and Electron Devices Directorate (ARL-SEDD)

In most research on distributed inference problems, sensor observations are assumed to be statistically independent or at least conditionally independent for analytical tractability. In the real world, however, observations are statistically dependent. One barrier in this area is the inability to accurately model statistical dependence in a form that can be used for information fusion to enhance inference performance. The goal of this research is to explore ways to accurately characterize statistical dependence and system diversity followed by creating computationally efficient approaches that can scale to large systems.

In FY16, Professor Varshney and his team established a new approach to distributed detection with dependent heavy-tailed signals. The new approach uses α-stable signal models with a copula-based dependence model to characterize dependent heavy-tailed distributions. The sensor signal model is general. It does not explicitly specify whether the phenomenon of interest is embedded in i.i.d. α-stable noise or if the α-stable model characterizes the dynamics of the phenomenon itself. The asymptotic behavior of copula model selection is characterized by the Kullback-Leibler distance metric. Research derived the asymptotic distribution for the probabilities of false alarm and detection. To evaluate its performance, this method was applied to a personnel detection problem utilizing the acoustic and seismic sensor dataset which was experimentally collected at the Army Research Laboratory. Experiments have shown significant improvement of this new approach (GLRT) over traditional methods of assuming independent signals (see FIGURE 5). This new approach has been transitioned to ARL-SEDD for sensor network based personnel detection for border security.
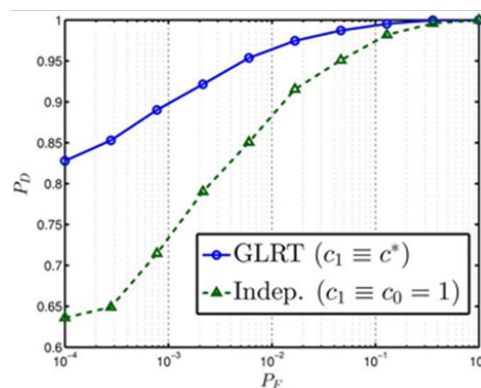

FIGURE 5
ROCs comparing the new method (GLRT) with independent signal modeling.

B. Fault Aware Intelligent Software for Exascale Systems
Investigator: Professor Robert Lucas, University of Southern California, Single Investigator Award
Recipient: DoD and DoE Laboratories

Today's standard model of computation, embodied in familiar programming languages, assumes that the underlying computer runs correctly. This model is generally accepted, except in safety critical systems like flight controls. In the near future, this will no longer be true due to the continued scaling of VSLI. In addition it will be prohibitively expensive to enforce total operational correctness with error correction using redundancy. The goal of this project is to design and implement software that exploits human knowledge of what faults are

significant, and what are not, to reduce the overhead of maintaining the illusion of perfect computing systems. This will save time and energy for large-scale Defense computations.

In FY16, Professor Lucas and his research team developed an assertion language that a knowledgeable user can use to assert what regions of a program's state space can tolerate errors so that these programs can continue to correct solutions. They also extended a standard programming Application Program Interface (API) to allow a knowledgeable user to be able to provide alternative repair strategies that will reduce the frequency of check-pointing and restarting, thus saving time and energy. They distributed versions of their assertion language to a DoD funded investigator, Professor Vivek Sarkar at Rice University, Dr. David Bernholdt at Oak Ridge National Laboratory, and Erik deBenedictis of Sandia National Laboratory. Also, they installed this language to a DoD computer center for use with an up-to-date release of the ROSE Compiler Infrastructure that supports their assertion language resilience directives at the direction of the Government.

C. Integrated Computer-Aided Cognitive Task Analysis
Investigator: Professors Peng Liu and John Yen, Penn State University
Recipient: ARL Computational and Information Sciences Directorate (ARL-CISD)

As cyber-attacks become more sophisticated, cyber-attack analysts are required to process large amounts of cyber related data (system status information, logs, and intrusion alerts) to determine whether a certain event is an ongoing attack attempt. Quite often they need to analyze and reason under various levels of uncertainties to capture a complete situation awareness framework (see FIGURE 6). Cyber Analysts' knowledge and experience play a significant role in successfully detecting cyber-attacks. The goal of this research is to capture and study the fine grained analysts' cognitive processes to help researchers gain a deeper understanding of how they conduct analytical reasoning, and elicit their procedural knowledge and experience to further improve their performance.
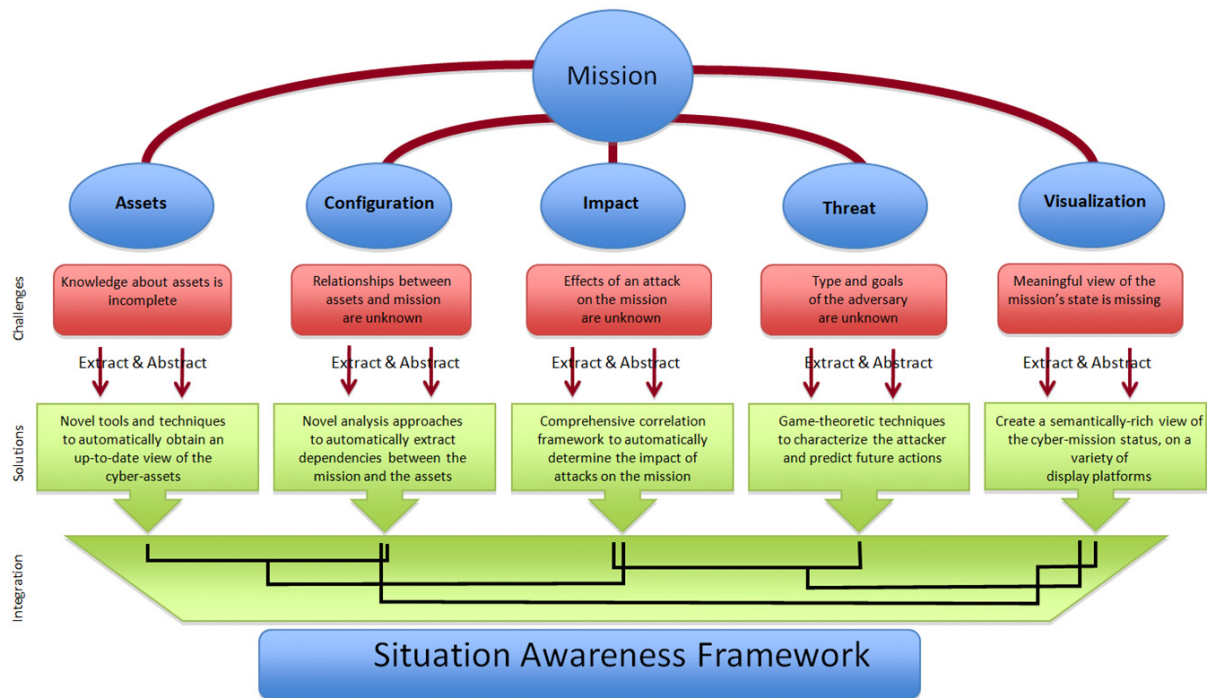

FIGURE 6

Cyber situation framework for attack analysis, prediction, and visualization. This research builds on results from the FY09-FY15 cyber situation awareness MURI project. This framework incorporates cyber assets, cyber configuration, attack impact, threat analysis, and situation visualization.

In FY16, the research team created an integrated computer-aided data collection method for cognitive task analysis (CTA). The CTA system has three building blocks: (1) a trace representation of the fine-grained cyber-attack analysis process, (2) a computer tool supporting process tracing, and (3) a laboratory experiment for collecting traces of analysts' cognitive processes in conducting a cyber-attack analysis task. This CTA method integrates automatic capture and situated self-reports in a novel way to avoid distracting analysts from their work and adding extra work load. The team has been working closely with cyber analysts and researchers from ARL-CISD in the field test of the CTA tool with more than 10 full-time professional analysts. The results of the preliminary trace analysis with ARL scientists indicate that this method may be a feasible way to gain understanding of how analysts perform cyber-attack analysis tasks, and it may provide promising contributions to analysts' for self-reflection, elicitation of their procedural knowledge, or for new tool development.

V.   ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Statistical Inference in the Compressive Domain
Professor Aswin C. Sankaranarayanan, Carnegie Mellon University, Single Investigator Award

The objective of this project is to solve classification and inference problems on dimensionality-reduced data, referred to as compressive inference. A key hallmark of compressive inference is the ability to directly obtain the compressed data using novel computational cameras. The main benefits of compressive inference are reduced storage, communication, energy, and processing costs since inference is performed directly on low-dimensional compressed data. A critical aspect is the identification of regimes where compressive inference can be effective, providing a theoretical analysis of the performance gains to be derived via compressive inference, and finally, demonstrating the practicality of the schemes over multiple datasets.

The benefits of compressive inference are demonstrated in scenarios where sensing and processing are costly. It is anticipated that research in FY17 will establish new compressive inference techniques for estimating material composition from infrared hyperspectral images as well as reflectance functions. Hyperspectral images have been widely used for inferring the presence of materials in a scene (for example, presence of minerals for mining, presence of chemicals in an adverse scenario, and oil leaks). However, detection at high fidelity requires very precise instruments that can sense at very high spectral precision, which requires long acquisition time as well as immense computational capabilities to process the high-dimensional data. The main goal of this research is to learn discriminative measurement codes that alleviate both challenges. The information on material composition will be augmented by reflectance functions which characterize surface properties like shine, smoothness/roughness, speckle, and sub-surface scattering. Such information is complementary to the spectral profile and hence, will lead to new methods for classification/discrimination of materials from visual information with improved reliability and accuracy of classification.

B. Establishing Principled Foundations for Honey Objects in Information Security
Professor Ari Juels, Cornell University, Single Investigator Award

Cyber deception is a proactive technique to manipulate the mental state and decision process of the adversary so that to degrade and mitigate their attack effectiveness. Honey objects, decoy resources used to lure, deflect, or detect adversaries in computer systems, are a powerful tool to distract and misguide potential attackers. Deception techniques such as honeypots have caught a great deal of interest in the past several years. In addition, honey objects have also been proposed and deployed for networks, databases, and cyber-physical systems to distract attackers. However, fundamental theories for deception techniques such as honey objects are still missing.

The objective of this research is to develop a theoretical framework for honey objects by applying formalisms from cryptography, including game-based security definitions and hardness reductions, to reason about the security of honey objects and illuminate their design space. Professor Juels and his team will couple theoretical exploration with a framework for empirical investigation and validation using statistical models. In addition, the team will uncover connections with related research domains, such as steganography and censorship evasion, show how techniques from statistics and machine learning can be recruited in the service of honey object construction, and enable rigorous security guarantees for honey objects informed by experimental results. It is anticipated that in FY17, the team will establish a scientific foundation by building upon the notion of distribution-transforming encoders (DTEs) in order to make conceptual connections among a range of different techniques including steganography, honeywords, and format-transforming encryption, among others.

C. Efficient Computational Models for Simulating Large-Scale, Heterogeneous Crowds
Professor Ming C. Lin, University of North Carolina - Chapel Hill, Single Investigator Award

Understanding the behavior of pedestrians in a crowded scene (see FIGURE 7) has been the subject of extensive research in multiple domains, including applied mathematics, robotics, psychology, sociology, civil and traffic engineering, architectural and urban design. Many applications such as training for battlefield simulation and urban warfare, intelligent surveillance, management of large mobs or unruly crowds, as well as use of robots in battlefields and dangerous environments need improved capabilities to simulate large crowds. Such crowds are characterized based on number of agents or pedestrians (e.g. large crowds with tens or hundreds of thousands of people), high densities, as well as heterogeneous or varying behaviors. The current state of the art is not able to model such large and diverse crowds that arise in different applications.
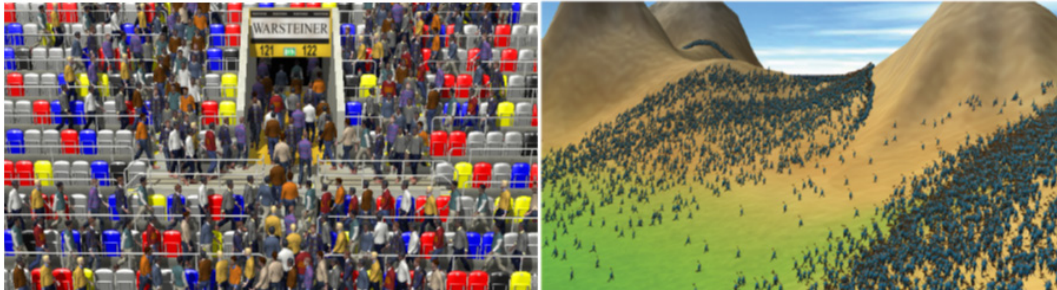

FIGURE 7

Complex crowd simulation benchmarks that will be used to evaluate performance. Stadium model (left) used to simulate evacuation and a battlefield simulation on an uneven terrain (right).

Motivated by the practical demands of modeling and simulation and better understanding of dynamic aggregate behaviors that are observed in modern-day Megacities, the goal of this project is to develop novel computational models and real-time crowd simulation algorithms that can be used for battlefield simulation, personnel training, and design evaluation. It is anticipated that in FY17, novel data-driven crowd simulation algorithms will be developed using Bayesian learning that exploit observed crowd behaviors captured using videos and other sensor data.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Cliff Wang
Division Chief
Program Manager, Information and Software Assurance

Dr. Mike Coyle
Program Manager, Computational Architectures and Visualization

Dr. Liyi Dai
Program Manager, Information Processing and Fusion

B. Directorate Scientists

Dr. Randy Zachery
Director, Information Sciences Directorate

Dr. Bruce West
Senior Scientist, Information Sciences Directorate

Ms. Anna Mandulak
Contract Support

C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 5: ELECTRONICS DIVISION

I.   OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2016* is to provide information on the programs and basic research supported by ARO in fiscal year 2016 (FY16), and ARO's mission to create basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Electronics Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and transitions facilitated by this Division in FY16.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of research in the ARO Electronics Division is to discover and control phenomena that involve charged particles and waves in solid state materials and plasma. More specifically, the Division supports basic research to discover and control stimulus-response properties of electronic materials/structures, to leverage nanotechnology for enhanced electronic properties, to comprehend and mitigate distortion and noise, to understand and exploit complex electromagnetic and acoustic phenomena and propagation, and to explore ultra-fast, solid state and plasma mechanisms and concepts. The results of this research will stimulate future studies and help keep the U.S. at the forefront of research in electronics by revealing new pathways for the design and fabrication of novel electronic structures that have properties that cannot be realized with current technology.

2. Potential Applications. Electronics research is relevant to nearly all Army systems; therefore, research under this program provides the underlying science for a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the full spectrum of the Army's "System of Systems." Army-relevant research in electronics spans areas such as (i) nano- and bio-electronics to provide components that interface with biological systems, enhance the creation and processing of information, and require less power (ii) studies in electromagnetics, acoustics, microwaves, and power to enable multimodal sensing for detection, identification, and discrimination of environmental elements critical to decision-makers in complex, dynamic areas , including defeat of electronic threat systems, (iii) optoelectronics, which involves the creation and use of electromagnetic radiation from far infrared to X-ray for sensing, communication as well as countermeasures to interrogate, disrupt, and defeat hostile infrared sensor systems and (iv) action-reaction relationships in electronic materials and structures that may lead to new devices and methods for sensing and communication over long ranges and within complex environments.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Electronics Division coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), as well as the various DOD Labs and other governmental activities with electronics research missions. Moreover, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, sensing is a research element of all ARO Divisions, and the Electronics Division serves as the focal point for ARO sensing research. Specific interactions include joint projects with the Physics Division that promote research for physics-based understanding of semiconductor materials, non-reciprocal materials and devices, propagation effects, plasma devices, and stimulus response effects in condensed matter. The Electronics Division also coordinates its research portfolio with the Materials Science Division to pursue the design and characterization of new materials and structures, the evaluation of electrical properties, and the study of electronic processes at the molecular level. This Division complements its research initiatives in the Chemical Sciences Division to

include research to understand how chemical changes and chemical structures influence electrical, magnetic, and optical properties and investigations of high frequency spectroscopic techniques for use in chemical defense, especially explosive detection. The Life Sciences Division's Program Areas also interface with electronics research in areas of biological detection as well as interfacing to biological organisms. Lastly, creating computational methods and models for target recognition and understanding nano-molecular structures and carrier transport shared research goals between the Electronics and Information Sciences Divisions.

In addition, extramural basic research in Electronics supports almost all of the other ARL S&T Campaigns, particularly the Materials Research Campaign which is supported by all of the Division's sub-areas with novel electronic and photonic materials. The Computational Sciences Campaign is supported through novel Nano, Bio, and Optoelectronic computing, Sciences-for-Maneuver by active and passive sensing, Information Sciences by new algorithms from biosciences as well as electromagnetic discoveries, Sciences for Lethality and Protection through targeting and directed energy, and Human Sciences through understanding and interfacing electronically with biological systems. The Electronics Division had 7 active cooperative agreements with these campaigns including a new cooperative agreement between the Materials Research Campaign and the State University of New York at Stony Brook to create novel metamorphic III-V narrow band structures.

B. Program Areas

The Electronics Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY16, the Division managed research within four Program Areas: (i) Nano- and Bio-electronics, (ii) Electromagnetics and Radio Frequency Electronics, (iii) Optoelectronics, and (iv) Electronic Sensing. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have long-term objectives that collectively support the Division's overall objectives.

1. Nano- and Bio-electronics. The program focuses on the creation of novel electronic devices including nano- and bio-based sensors and transducers based on semiconductor electronics and hybrid molecular-semiconductor devices in addition to organic-inorganic hybrid materials. This project supports basic research that will apply biology concepts to electronics and photonics to create biomimetic structures and devices for information processing, information storage, electronic components, and actuators. It will also create unique electronic sensors at the nano to the macro level that interface with biological materials in order to extract information on biological systems. The long term goal of this task is to discover and control novel phenomena by the combination of electronics, photonics, and bioscience to provide novel electronic technological capabilities for defense-related applications such as sensing, data processing, communications, target recognition, navigation, and surveillance.

2. Electromagnetics and Radio Frequency Electronics. This program area is concerned with investigation of electromagnetic (EM) and radio frequency (RF) phenomena for integrated antenna arrays, multifunctional antennas, EM power distribution, and new sensing modalities. It also explores acoustic phenomena and new concepts for circuit integration for greater functionality, smaller size/weight, lower power consumption, enhanced performance, with focus in the frequency regime from low to terahertz frequencies.

This area addresses the science behind new approaches to the generation, transmission, and reception of EM power and signals. Emphasis is placed on the HF through terahertz spectrum, however, novel ideas at lower frequencies down to direct current may be addressed. In the RF regime orders of magnitude improvements in systems performance, cost, weight, reliability, size characteristics, and functionality will be sought. Issues include the coupling of EM radiation into and out of complex structures, antennas, both active and passive, transmission lines and feed networks, power combining techniques, EM wave analyses of electrical components, and EM modeling techniques. Thermal problems stemming from the concentration of higher and higher power into smaller and smaller volumes will be addressed. Antenna research will break away from the methodologies that were developed for continuous-wave, narrowband, steady-state operation to invent new design techniques, architectures, and materials that can dramatically increase the radiation efficiency and bandwidth of tactical antennas while simultaneously reducing their size and signature. The EM and acoustic detection and analysis of underground targets, landmines, and IED's will continue to be of interest. Unusual propagation effects in the

atmosphere and gaseous plasmas offer new opportunities for sensing and detection. Army applications of this technology include communications (both tactical and strategic), command and control, reconnaissance, surveillance, target acquisition, and weapons guidance and control.

3. Optoelectronics. The goal of this Program Area is to discover and control novel nanostructure and heterostructure designs for the generation, guidance, and control of optical/infrared signals in both semiconductor and dielectric materials. The research in this program may enable the design and fabrication of new optoelectronic devices that give the Soldier high-data-rate optical networks including free space/integrated data links, improved IR countermeasures, and advanced 3D imaging. This program has three Thrust areas: (i) High Speed Lasers and Interconnects, (ii) Ultraviolet and Visible Photonics, and (iii) Mid-infrared Lasers. The research topics seek to overcome slow spontaneous lifetimes and gain dynamics, low carrier injection efficiency, poor thermal management, and device size mismatches. Novel light emitting structures based on III-V compounds, wide bandgap II-VI materials, rare-earth doped dielectrics, and silicon nanostructures are being investigated along with advanced fabrication and characterization techniques. Nanotechnology is exploited to allow interfacing of optoelectronic devices with electronic processors for full utilization of available bandwidth. Electro-optic components are being studied for use in guided wave data links for interconnections and optoelectronic integration, which are all requirements for high speed full situational awareness. In addition, emitters and architectures for novel display and processing of battlefield imagery are also important.

4. Electronic Sensing. The goal of this Program Area is to extend the underlying science behind action-reaction relationships in electronic materials and structures as well as understand target signatures. This Program Area is divided into two research Thrusts: (i) Photonic Detection and (ii) Thermal, Mechanical, and Magnetic Effects. The scientific objective of Photonic Detection is to understand and control the direct conversion of light to charge in infrared materials and structures. This includes the design and fabrication of novel detector structures, such as superlattice or barrier structures, as well as novel plasmonic effects. An important element in this thrust area is the reduction of performance limiting defects in semiconductor material and structures through lattice matching and other methods. Development of novel characterization techniques is also explored to determine the fundamental issues behind carrier transport, lifetimes, and noise. The Thermal, Mechanical, and Magnetic Effects Thrust includes the modalities of acoustic, magnetic, infrasound, as well as thermal effects for infrared detection. Research in this Program Area seek to give the Soldier 100% situational awareness of vehicles, personnel, weapon platforms, projectiles, explosives, landmines, and improvised explosive devices (IEDs), in day/night, all weather, and cluttered environments through natural and man-made obstructions.

C. Research Investment

The total funds managed by the ARO Electronics Division for FY16 were $21.4 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $6.7 million and $1.0 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $1.9 million to projects managed by the Division. The Division also managed $1.8 million of Defense Advanced Research Projects Agency (DARPA) programs, and $2.3 million provided by other Federal agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $5.8 million for contracts. In addition, $1.9 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.4 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY16 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY16 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY16, the Division awarded 22 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Norman Armitage, Johns Hopkins University; *Thz Measures of Axion Electrodynamics and Exotic Superconducting Interfaces in Topological Insulator Films and Their Heterostructures*

- Professor Dennis Deppe, University of Central Florida; *Scalable High Speed Laser Diode for Silicon Integration*

- Professor Dmitri Donetski, Research Foundation of SUNY at Stony Brook University; *Novel Metamorphic Heterostructures for Long Wave Infrared Optoelectronics*

- Professor Yeshaiahu Fainman, University of California - San Diego; *Optoelectronic Technology for Nanosecond WDM-Based Chip-Scale Optical Networking*

- Professor Timothy Havens, Michigan Technological University; *Heterogeneous Multisensor Buried Target Detection Using Spatiotemporal Feature Learning*

- Professor Hongxing Jiang, Texas Technical University; *Deep UV Emitters and Polariton Lasers*

- Professor Mercedeh Khajavikhan, University of Central Florida; *Design, Fabrication, and Characterization Of Electrically Pumped Coaxial Nanoscale Lasers*

- Professor Jian Li, University of Florida - Gainesville; *Enhanced UWB Sensing Via RFI Mitigation and Missing Data Recovery*

- Professor Zhaolin Lu, Rochester Institute of Technology; *Ultracompact, High-Speed Field-Effect Optical Modulators*

- Professor Luke Mawst, University of Wisconsin - Madison; *QD Lasers Employing Full Three-Dimensional Active Region Carrier Confinement*

- Professor Daniel Mittleman, Brown University; *Terahertz Metasurfaces for Wavefront Control and Waveform Synthesis*

- Professor Mina Raieszadeh, University of Michigan - Ann Arbor; *Exploring Ultimate Limits of Energy Dissipation in Wide-Bandgap Semiconductors*

- Professor Shriram Ramanathan, Purdue University; *Mott Transistor: Fundamental Studies and Device Operation Mechanisms*
- Professor Vivek Shenoy, University of Pennsylvania; *Strain Engineered Topological Phases of 2D Materials and Their Heterostructures*
- Professor Volker Sorger, George Washington University; *2D Material-Based Electro-Optic Modulation on a Silicon Platform*
- Professor Dmitri Strukov, University of California - Santa Barbara; *Spatial-Temporal Memory Effects in Nanoelectronic Neuromorphic Networks*
- Professor Han Wang, University of Southern California; *Two-Dimensional Material Based Synaptic Devices for Neuromorphic Computing*
- Professor Judy Wu, University of Kansas; *Fundamental Physics of Carbon-Based Nanyhybrids for High-Performance Infrared and Ultraviolet Detection*
- Professor Boris Yakobson, William Marsh Rice University; *Computational Design Of Stacked Heterostructures From Low-Dimensional Materials For Strategic Applications*
- Professor Amnon Yariv, California Institute of Technology; *Investigation of Dynamic Effects and Coherence Limits of Hybrid Si/III-V Lasers*
- Professor Robert York, University Of California - Santa Barbara; *Epitaxial Cd3As2 For RF Device Applications*
- Professor Yong Zhang, University Of North Carolina - Charlotte; *Correlative Study of Defects in Semiconductors*

2. Short Term Innovative Research (STIR) Program. In FY16, the Division awarded 15 new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Les Atlas, University of Washington; *Alternatives To Digital Processing and Demodulation for Standoff Sensors*
- Professor Ganesh Balakrishnan, University of New Mexico Albuquerque; *Two-Step Etch Process for Fabrication of III-V Nanolasers*
- Professor Bjorn Birnir, University of California - Santa Barbara; *The Chaotic Quantum Oscillator*
- Professor Gregory Carman, University of California - Los Angeles; *Spin Waves Generated by Elastic Waves*
- Professor Yeshaiahu Fainman, University of California - San Diego; Optoelectronics: *Low-Energy Tunable Self-Modulated Nanolasers*
- Professor Saniya LeBlanc, George Washington University; *Next Generation Additive Manufacturing: Laser Sintering & Melting of Thermoelectric Materials*
- Professor Zetian Mi, McGill University; *Molecular Beam Epitaxial Growth and Characterization of Two-Dimensional BN/Mo$_x$W1-xSe$_2$ Heterostructures*
- Professor Jagdish Narayan, North Carolina State University; *Doping of Diamond beyond Thermodynamic Solubility Limit for Electronic Applications*
- Professor Ram Narayanan, Pennsylvania State University; *High-Resolution Radar Waveforms Based on Randomized Latin Square Sequences*
- Professor Seth Putterman, University of California - Los Angeles; *Non-Contact Ultrasonic Imaging*
- Professor Sayeef Salahuddin, University of California - Berkeley; *Electronic Probing of NV Centers using Spin-Spin Interactions for Ultra-Sensitive Imaging and Frequency Synchronization*
- Professor Michael Steer, North Carolina State University; *Exploration and Discovery of Signals in the Analog Domain*
- Professor Michael Stroscio, University of Illinois - Chicago; *Tailoring Vibrational Modes and Interactions in Resonators and Waveguides: Multiscale Model of Phonon and Phonon Interactions - Transition from MEMS to NEMS*

- Professor Yuanxun Wang, University of California - Los Angeles; *Broadening the Efficiency Bandwidth Product of Electrically Small Antenna through Direct Antenna Modulation (DAM) Transmitting*
- Professor Daniel Wasserman, University of Texas - Austin; *Coupling Optical Phonons to Free Space Photons*

3. Young Investigator Program (YIP).

No new starts were initiated in FY16.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY16 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Workshop on Semiconductor Platforms for Synthetic Biology and Hybrid Bioelectronic Systems*; Atlanta, GA; 22-23 February 2016
- *Frontiers of Neuromorphics*; Los Angeles, CA; 2-4 April 2016
- *17th IEEE International Vacuum Electronics Conference*; Monterey, CA; 19-21 April 2016
- *71st International Symposium on Molecular Spectroscopy*; Urbana-Champaign, IL; 20-24 June 2016
- *International Conference on Metalorganic Vapor Phase Epitaxy*; San Diego, CA; 10-15 July 2016
- 2016 Lester Eastman Conference on High-Performance Devices; Bethlehem, PA; 2-4 August 2016
- *OSA Science and Applications of Nanolasers Incubator*; Washington, DC; 7-9 September 2016
- *OSA Subwavelength Photonics Incubator*; Washington, DC; 21-23 September 2016
- *2016 International Conference on Infrared, Millimeter, and Terahertz Waves*; Copenhagen, Denmark; 25-30 September 2016

5. Special Programs. In FY16, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded five new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Electronics Division; therefore, all of the Division's active MURIs are described in this section.

1. Near and Far-Field Interfaces to DNA-Guided Nanostructures from RF to Lightwave. This MURI began in FY10 and was granted to a team led by Professor Peter Burke at the University of California - Irvine. The goal of this research is to develop new sensing modalities for chem/bio sensing based on materials development in nanotechnology and nanoscience, and to interface nano-electronic and nano-optical components to biologically relevant physical properties.

In order to tap the requisite contributions from different academic disciplines (DNA chemistry, electrophysiology, nano-electronics, optics and THz spectroscopy), three sensing hardware testbeds are being developed for further testing, functionalization, and analysis: (i) bottom up carbon electronics (graphene, nanotubes); (ii) top down silicon nano-electronics (top down Si nanowires); and (iii) nano-optics (CdSe and other nanowire emitter/detector architectures). Two functionalization schemes are being be applied to these testbeds to enable sensing: DNA origami aligned to nanowire arrays and ion channel functionalization for electrophysiology at the nanoscale. Unique aspects of this sensing research include multiplexing (massively parallel sensor arrays) via DNA self-assembly. Using this approach, in principle, each nanowire in an array can have a different sensing functionality, at unprecedented pitch. In addition, direct integration of bio-electrical signals (ion channel currents) to nano-electrodes (carbon, silicon, and nano-optics) are being explored. A key discovery in the recent year is that the ion channel current pulses can be used to charge the quantum capacitance

of graphene, demonstrating a qualitatively new sensing modality for nanoscale electrophysiology. Lastly, single-molecule sensitivity and novel mechanisms for selectivity at THz frequencies are being pursued. Advances in this MURI will enable a new class of sensors for applications in biomedical diagnostics for civilian and warfighter health care, chemical agent detection, nano-optical devices for sensing, and neural-electrical interface at unprecedented spatial resolution.

2. Defect Reduction in Superlattice Materials. This MURI began in FY11 and is led by Professor J. M. Zuo at the University of Illinois - Urbana Champaign. The team consists of researchers from Arizona State University, Georgia Tech, and the University of North Carolina - Charlotte. The objective of this project is to determine and understand the relationship between minority-carrier lifetimes and classes of defects in superlattice materials and to formulate strategies for growth and post processing to eliminate or mitigate defects.

This research effort includes an in-depth study of the origins and structural, electrical and optical properties of defects, in-situ and ex-situ probing of defects during growth and fabrication, an investigation of defect reduction techniques, a study on ways to minimize the impact of defects on performance, and testing of results through fabrication and characterization of superlattice structures and devices. Understanding defects at the basic level in these superlattice materials will promote advancements in lasers and modulators as well as infrared detectors. For detectors, lifetime improvements will allow the next generation of focal plane arrays with increased long wave resolution, much larger array formats, broader spectral range into the very long wave infrared, and higher operating temperature to reduce life cycle costs.

3. Spin Textures and Dynamics Induced by Spin-Orbit Coupling. This MURI began in FY16 and is led by Professor Kang Wang at University of California, Los Angles. The team consists of researchers from University of California, Irvine, California Institute of Technology, University of Nebraska, North Carolina State University, and University of Texas, Austin. The objective of this project is to strive for understanding of interfacial spin-orbit coupling (SOC) and exchange coupling in novel heterostructures and superlattices of topological insulators (TIs), 2D transition metal di-chalcogenides (TMDs), and ferro-(FM)/ferri-/antiferro (AFM)-magnetic materials. High quality heterostructures and superlattices containing TI/TMDs, TI/FM, and TI/AFM with the atomically sharp interface are to be synthesized and characterized, and these will constitute an ideal laboratory for enabling understanding of the interfacial SOC effects and relevant spin textures and dynamics.

This project will exploit the symmetry breaking and SOC-induced collective properties (i.e., magnetization, spin wave, and spin-orbit torque) in these heterostructures and superlattices to realize new types of topological matters such as magnetic Skyrmions, topological valley insulators, and topological spin wave (magnonic) crystals. It will also help facilitate the development of new emerging fields including spin-orbitronics, spin-valley-tronics, and axion electrodynamics. In addition, direct electrical field manipulation of spin or magnetization textures in these proposed systems through spin-orbit torque and magnetoelectric effects will be investigated for energy efficiency. The anticipated results of this project will broaden understandings of the fundamental science enabled by SOC, and establish suitable material frameworks for new spin-orbitronic devices in which multi-functional applications of spintronics for ultra-low power electronics at terahertz can be realized. This research will set a milestone in the spin-based applications by creating the knowledge base to enable novel, fast, and energy efficient technologies for communications and information processing.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES. In FY16, the Division managed eleven new-start SBIR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of seven Phase I contracts and, four Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY14 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES. In FY16, the Division managed

nine new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of four Phase I contracts and five Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY14 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY16, the Division managed two new ARO (Core) HBCU/MI projects, and three new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY16.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY16, the Division managed nine new DURIP projects, totaling $1.3 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. JTO Multidisciplinary Research Initiative (MRI) Programs in High Energy Lasers

ARO currently manages eight MRI programs for the High Energy Laser Joint Technology Office (HEL-JTO) in Albuquerque (managed by OSD). Five of those are 2012 start MRIs and three of those were awarded through ARO's Electronics Division (the others through Materials and Physics). The three 2010 starts MRI are led by professors at Clemson University, the University of New Mexico, and the University of Central Florida. The latter two ended in FY16; whereas, the Clemson effort was extended an additional 2 years to further study the potential of all-solid photonic bandgap fibers. The two that ended were on high energy laser coatings and characterization techiques, and volume Bragg gratings. The 2012 start MRIs that are still active are led by professors at Rutgers, Texas Tech, University of California – Riverside, Clemson, and the University of Central Florida (Center for Research in Electro-Optics and Lasers). These MRIs are on the following topics: single crystal fiber lasers, rare-earth doped GaN, polycrystalline AlN ceramic gain media, leaky wave and gas-filled hollow-core fiber lasers, and nonlinearity mitigation in fiber lasers. The 2012 start MRIs are all in the final two years. ARO continues to play a significant role in leading the MRI programs by organizing kickoff meetings and program reviews, particularly in conjunction with the HEL-JTO Advanced Concepts Technical Area Working Group which leads the more basic research endeavors that HEL-JTO supports. The ARL Materials Science Campaign (ARL-CISD and ARL-SEDD) participate in HEL-JTO program evaluation through annual reviews.

I. DARPA Advanced Wide FOV Architectures for Image Reconstruction and Exploitation (AWARE)

The AWARE program focuses on technologies to enable wide FOV, higher resolution and multi-band imaging for increased target discrimination and search in all-weather day/night conditions. The Electronics Division coordinates research with this program by identifying and monitoring basic research projects with complementary goals. In FY16, the AWARE program provided new funding for four university projects because of ARO's leadership in the area of infrared photodetectors. In one, the objective is to create low-cost zero-dimensioned nanostructure-contained quantum disks that can be integrated into uncooled LWIR focal plane arrays. Another will demonstrate that the extreme mobility of CdO will enable plasmonic uncooled mid-infrared detectors. The third will determine the causes of Random Telegraph Noise and use that information to design

read out integrated circuits in advanced fabrication nodes. The fourth will create and test efficient modulators that can achieve over 1 GHz bandwidth for SWIR (short wave infrared) Time of Flight (ToF) imaging. These follow ARO MURIs on quantum dot photodetectors and uncooled thermal materials as well as single investigator projects on noise and plasmonic enhancements for better photonic properties.

J. DARPA Low Cost Thermal Imaging – Manufacturing (LCTI-M)

The Low Cost Thermal Imager - Manufacturing (LCTI-M) program seeks to enable widespread use of infrared imaging technology by individual warfighters and insertion in small systems. The Electronics Division coordinates research with this program by identifying and monitoring basic research projects with complementary goals. In FY16, the LCTI-M program provided additional funding for an ongoing project to create free standing bolometer structures with thinner layers, lower heat capacity, and improved imaging performance over existing structures by use of atomic layer deposition. This was a joint project with the University of Colorado and DRS Technologies. ARO is the technical monitor for this project because of its leadership of an ARO MURI concerning uncooled materials.

K. DARPA Efficient Linearized All-Silicon Transmitters ICs (ELASTx) Program

The goal of the ELASTx program is to enable monolithic, ultra-high power efficiency, ultra-high linearity, millimeter-wave, silicon-based transmitter integrated circuits (ICs) for next-generation military microsystems in areas such as radar and communications. The ARO Electronics Division currently co-manages two university grants within this program that are exploring quasi-optical power combining of Doherty amplifiers, and asymmetric multilevel outphasing of large numbers of transistor amplifiers. The program will lead to revolutionary increases in power amplification efficiency while simultaneously achieving high linearity for digitally modulated signals. Prototype ELASTx amplifiers are being tested by scientists in ARL-SEDD for potential use in Army radar and communications systems.

L. DARPA Microscale Plasma Device (MPD) Program

The goal of the MPD program is to support fundamental research in the area of microplasma device technologies and substrates for operation in extreme DoD-relevant environments. The ARO Electronics Division currently co-manages two grants within this program that will develop fundamentally new fast-switching microplasma devices, develop modeling and simulation design tools, and demonstrate the generation of a plasma with an extremely high charge density (1020 - 1022 unbound electrons per cubic centimeter) in a sealed cell with solid walls. This charge density is four to six orders of magnitude larger than is achieved in current microplasma research and is comparable to the carrier density in metallic materials. Research results will be communicated to ARL-SEDD Electronics Technology Branch scientists in order to identify opportunities for technology transfer. If successful, the MPD program will provide proof-of-concept for fast-switching microplasma devices that may enable new sources of radiated energy at sub-millimeter wave and terahertz frequencies, the enabling science behind new high resolution imaging radar and covert communication systems.

M. DARPA High Frequency Integrated Vacuum Electronics (HiFIVE) and THZ Electronics Programs

The long-term vision for the DARPA THZ Electronics program is to develop the critical device and integration technologies necessary to realize compact, high-performance electronic circuits that operate at center frequencies exceeding 1012 cycles per second (i.e., 1 THz). The DARPA HiFIVE program will develop a compact, efficient source of electromagnetic energy capable of generating 100 W with 5 GHz bandwidth at 220 GHz using innovative cold cathode and micromachining technologies. The ARO Electronics Division and ARL-SEDD Electronics Technology Branch co-manage projects within these programs with a goal of using silicon micromachining and MEMS processes to produce precision interaction structures scaled for these extremely small wavelengths. These programs have a high potential impact on military communications, ECM, and radar systems. Two of the HiFive projects managed by ARO have now ended.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Electronics Division.

A. Double Tunnel Injection Quantum Dot Lasers
Professor Levon Asryan, Virginia Tech University, Single Investigator Award

Professor Levon Asryan continued to make headway in understanding the dynamics of semiconductor quantum dot lasers. Specifically, the goal of this research is to investigate the potential of tunneling heterostructures to enhance the modulation bandwidth. Previous heterstructure approaches have both experimentally and theoretically shown modulation bandwidths of up to 7.5 GHz. In FY16, the research team successfully demonstrated the possibilities for 20 GHz 3 dB (half-power) modulation bandwidths, or equivalently, 40 Gb/s data rates by using Professor Asryan's more thorough modeling which allows for tunneling of both electrons and holes into the quantum dots shows (see FIGURE 1). Such understanding can be applied to multiple material systems and devices as well as laser cavity regimes. In particular, much smaller lasers and laser cavities than edge-emitting lasers hold relevance to the low energy and high-speed program thrust of this endeavor. Both nanolasers and vertical cavity surface emitting lasers can incorporate such heterostructures for short distance interconnects that may soon be incorporated into computational platforms to revolutionize computer communications.
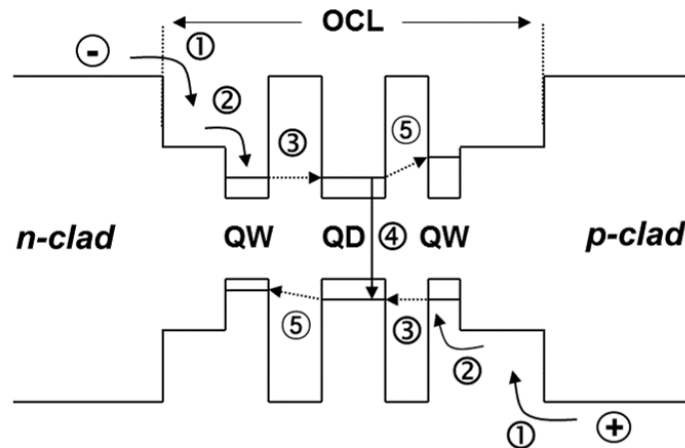

FIGURE 1
The numbers and diagrams show how various carrier transport elements are individually considered and utilized in studying the various aspects of whether higher modulation speeds can be attained.

The work of Professor Asryan to explore the ultimate limits in modulation speed of quantum dot lasers had a number of aspects to it. Both conventional strain induced (Stranski-Krastanow) quantum dots and lithographic or etched quantum dots could be incorporated in the models. Realistic carrier capture and emission times as well as transport times were studied. For carrier capture times below 1 ps and tunneling injection times below 0.1 ps which are "fast enough" for typical diode laser regimes, the 20 GHz modulation bandwidth quoted already is still achievable (see FIGURE 2). Why such speeds have not been achieved then already comes back to the materials epitaxy science. Knowing these results are possible though may influence the studies of material sceintists in terms of pushing the limits of various semiconductor alloy material systems to achieve both electron and hole (double-sided) tunneling injection. Another reason one may want to know such results is to motivate new heterostructure design and nanofabrication techniques. Both 2D and nanomembrane materials are under intense investigation including heterostructure formation, of late, toward making devices with new properties. Those properties include achieving band-offsets that are difficult to achieve with standard crystal growth epitaxy. These results may be utilized to guide the fabrication and design goals toward making much faster quantum dot lasers. For example there is continued interest in new techniques to make quantum dot lasers on silicon.

Although clock speeds of 7.5 GHz are sufficient currently compared to microprocessor speeds, off-chip clock rates with multiplexed signals could be much faster and photonic integrated circuits that operate in various functionalities (such as for new optical computing studies) may desire to move toward the 20 GHz speeds. Quantum dot lasers are generally of such high importance in low energy nanophotonics due to their record low threshold current densities- a key factor in reducing total energy consumption.
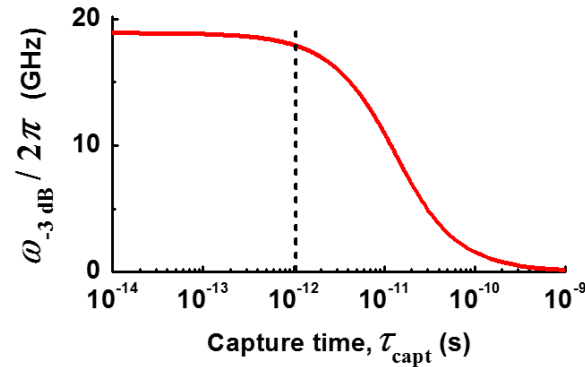

FIGURE 2

Double Tunnel Injection Quantum Dot Laser modulation bandwidth as a function of carrier capture time.
Realistic carrier capture times are less than 1ps indicating the 20 GHz speed is possible via double-sided tunneling.

B. Topological Insulators for Novel Device Applications
Professor Ki Wook Kim, North Carolina State University, Single Investigator Award

The goal of this project is to exploit the unique characteristics of topological insulator (TI) based structures for highly functional devices beyond the limits of the current state of the art. In FY16, the research team successfully analyzed the nonlinear dynamics of the TI-magnet system and demonstrated an energy efficient process/mechanism for magnetization switching and persistent oscillations via a DC electrical bias. Extending the work reported earlier that was based on the coherent tunneling model, the investigation comprehensively examined the mutually dependent interactions between the TI surface states and a ferro-magnet under more realistic electron transport conditions.

When an electrical current flows in the TI surface region interfaced with a magnetic material, the resulting natural spin polarization modulates the magnetization via the effective torque. Conversely, the reoriented magnetization affects the TI surface current (both the intensity and spin polarization) through the electronic band modification. To account for these self-consistent responses in the cases of non-coherent electrical conduction on the TI surface, an empirical approach was adopted based on the experimental and theoretical findings available in the literature concerning the anomalous Hall current, which turned out to be very crucial for the nonlinear magnetization dynamics (see FIGURE 3). A key finding is that an entire range of the responses, such as reversal and auto-oscillations (with the frequencies in the GHz), are possible, even for diffusive cases, by simply adjusting the material and excitation conditions. One unexpected behavior is the possibility to anti-align the magnetization with respect to the effective field of the driving current. In other words, the magnetization may end up with the –y orientation even though the driving current induces a field along the +y axis via spin-momentum interlock. This scenario happens when the anomalous Hall effect becomes very pronounced and the resulting anti-damping effect dominates over the Gilbert damping term, which may turn out to be an artificial case. The PI has also examined the ballistic but incoherent case. The analysis revealed that the magnetization dynamics remain very similar to the diffusive case; except that the required voltages are now smaller due to the negligible resistance (thus, potential drop) in the channel. Compared with the previously reported coherent transport, the overall picture is again very consistent. The investigation clearly indicated that the desired magnetic behaviors such as reversal and persistent oscillation can be achieved under broad regimes of TI surface electron transport with a simple DC electrical control. With a minimal energy requirement as low as tens of atto-joules, the proposed mechanism offers an efficient alternative to the spin transfer torque or spin-Hall based approaches for potential magnetic memory/logic.
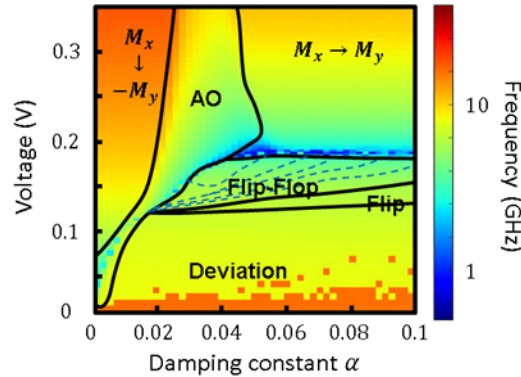
FIGURE 3

Simulation results with diffusive transport assumed in the interface region. A Magnetization dynamics mapped on the electrical bias (V)–Gilbert damping constant (☐) parameter space. The diffusive transport is assumed for the TI surface electrons. The solid lines separate the different dynamical regimes, while the dashed lines in the flip-flop region indicate the smeared nature of the boundaries between the two final states (+x or −x) after the precession. The background color provides the corresponding frequency of the magnetization rotation. AO stands for auto (or persistent) oscillations.

C. Fundamental Limitations on Phased Array Elements
Professor Do-Hoon Kwon, University of Massachusetts - Amherst, Single Investigator Award

Single isolated antennas have well established theoretical limitations depending on their structure and size. The goal of this research was to explore for the first time the limitations on planar phased arrays. In FY16, Professor Kwon's laboratory successfully developed a new theory based on the Lorentz reciprocity theorem, relating the receiving properties of infinite planar array elements (vector effective height and receiving area) in terms of their transmitting performance parameters. A new directivity quantity was introduced to describe the bidirectional and unidirectional nature of the radiation under any given scan condition. The exact expression for the receiving area was given for the first time. The contributing factors were found to be the radiation efficiency, the polarization and mismatch factors, and the Floquet directivity together with the projected element cell area in the scan direction. The fundamental upper bounds on the element matching bandwidth were derived for the first time. Quantitative element bandwidth bounds were found in terms of the strengths of the induced electric and magnetic dipole moments, taking into account the coupling between neighboring elements. For both resonant narrowband and ultrawideband responses, the bandwidth upper bounds were expressed in terms of geometrical (unit cell dimensions, scan angle, polarizabilities) as well as electrical (radiation efficiency, polarization mismatch factor, Floquet directivity, polarizabilities) design parameters. It was shown that smaller unit cell dimensions and strong induced dipole moments increase the bandwidth upper bound (see FIGURE 4). This new quantitative understanding of the interaction of design parameters in phased arrays will have a significant impact on the capability to quickly design highly efficient antenna arrays.
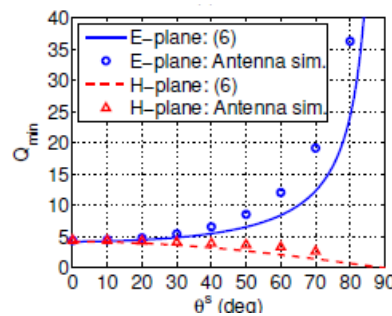

FIGURE 4

Q of a Dipole Array with Respect to Scan Angle. Fractional bandwidth = 1/Q.

D. Photon Statistics and Spectral Selectivity Limits of Thermal Detectors
Professor Joseph Talghader, University of Minnesota, Single Investigator Award

The objective of this research is to determine the effects of spectral selectivity on the photon statistics and the spectral limits of thermal detectors. The scientific theory that describes thermal infrared detectors was developed several decades ago for devices with uniform spectral absorption. In that body of work, the photon statistics of the detector was usually handled speciously, although since the number of modes in a typical thermal emission process is vast, the errors were negligible as Bose-Einstein contributions average out when integrated over many modes, leaving only standard Poisson statistics. Historically, since almost all thermal emission occurred in systems with large numbers of modes, it has not been important to have a quantitative model of photon statistics that incorporates Bose-Einstein contributions; however, the errors become significant for thermal detectors in high spectral confinement, i.e. small number of modes. These effects are becoming more important for various applications involving narrowband thermal detection, as well as coherent thermal emission and cavity quantum electrodynamics.

In FY16, Professor Talghader successfully discovered an exact general result for thermal photon population fluctuations for any average number of photons in any number of modes with any spectral dependence. His method sidesteps many of the mathematical complexities of previous treatments and produces a closed form analytic result. Using this, he further showed that the Bose-Einstein contributions could be significant in real detectors with high spectral confinement. This work could lead to hyperspectral thermal detectors that have higher sensitivity (due to less noise) and less uncertainty in the spectral resolution. In addition, the innovative method used in finding the analytical solution could be used to solve further unresolved questions in mathematics and other scientific fields.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Vertical Cavity Surface Emitting Laser based Transceivers for Optical Interconnects
Investigator: Dr. Charles Kuznia, Ultracommunications, Single Investigator Award
Recipient: Lockheed Martin, ARL-SEDD, ARL-CISD

Fiber optic micro-transceivers with improved ruggedness, temperature range of operation, and built-in-test (BIT) capabilities were developed thru ARO STTR investments at Ultracommunications. The micro-transceiver represents a platform for devices of various types that address array of Army technology needs. To specialize the functionality an ASIC (Application Specific Integrated Circuit) within the transceiver is programmed at low-power and low data-rate or high-data rate as well as analog or digital. The microtransceiver technology has the following features: (i) a method of coupling light between a VCSEL and fiber over wide temperature ranges, (ii) high-fidelity electrical pathways that will enable data rates beyond 40 Gbps (digital) or 40 GHz RF photonic links, (iii) an extremely compact package with a 'top-down' removable fiber connector, which can be soldered to the PCB (without an electrical connector), and (iv) potential for low cost with the use of component produced at the wafer scale.

Prior SBIR programs at Ultracommunications (including an ARO SBIR) aided in the development of ruggedized optical transceivers based on VCSEL (Vertical Cavity Surface Emitting Laser) transmitters. Further development ensued including development of a military standard for photonic packaging and ruggedization led by working groups chaired by Ultracommunications (a pioneer in military photonic interconnects). Then, in 2011, a follow-on STTR program was developed which aimed to further reduce the size and cost with a reduced number of parts as well as increased speeds, based on further improvements in the VCSELs. Now, in 2016, immediately following the phase II, with the management of ARO, ARL-SEDD and ARL-CISD, the transceivers have met military qualifications (see FIGURE 5).
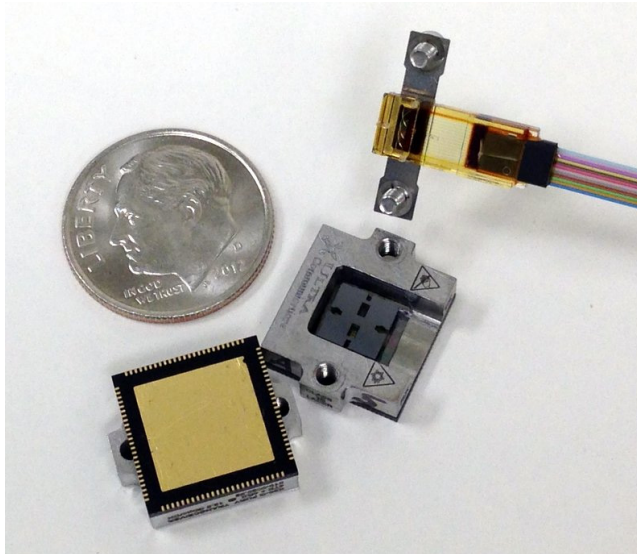

FIGURE 5
Optical transceiver. New Ultracommunications optical transceiver with built in test capability.

This technology is transitioning through commercial product sales to prime contractors responsible for advanced development of fiber optic systems. The product is baselined into programs for the high performance imaging with in terrestrial and airborne applications.   The product is under-going a qualification program was vetted

across multiple platforms to expand the suitability with retro-fit and next-generation fiber optic network installations and upgrades. The sales of this product ha**ve** resulted in over $1.1M in direct sales to 17 distinct customers, and $2.5M in follow-on government programs.

These modernized fiber optic transceivers with BIT capability increase the availability and performance of Army tactical weapons. The incorporation of BIT functionality within the fiber optic network reduces maintenance time, and allows rapid mission re-provisioning (changing the equipment on the vehicle to optimize for a mission). This increases the overall aircraft performance (mission-time vs. downtime) and weapons availability. This technology offers a significant improvement in available network bandwidth. The systems can also improve weapon accuracy with higher resolution imaging, and reduced lag in real-time video systems.

B. PN Nanojunctions in Compound Semiconductors
   Investigator: Professor Gary Wicks, University of Rochester, Single Investigator Award
   Recipient: Amethyst Research, Inc.

The goal of this research is to determine the important electronic phenomena at nano-scale dimensions and design nano-sized infrared detectors. Part of this project concerned research into unipolar barrier concepts leading to new infrared detector designs that were patented and licensed to Amethyst Research, Inc. for further development. A unipolar barrier is a heterostructure designed so that one carrier type, either electrons or holes and either minority or majority carriers, may flow unimpeded while the other carrier type is blocked. Professor Wicks started with the premise that unipolar barriers can be inserted into photodetector epitaxial structures to eliminate any dark current components with spatial makeups different than that of the photocurrent but no barrier structure can block currents generated in the absorber without also blocking the photocurrent, thus unipolar barriers cannot be employed to reduce Auger or diffusion currents. On the other hand, tunneling (both trap-assisted and band-to-band) currents, Shockley–Read-Hall currents, and surface currents have spatial makeups that are different than that of photocurrent, and thus can be blocked by proper use of unipolar barriers. His patents showed how to best place barriers for optimal performance. In particular, he showed that nBn and pBp structures (B is the barrier) have different applications. nBn devices should be employed when the surface conduction of the material is n-type and must use an optical absorber that is n-type. The pBp architecture should be employed when the surface conduction of the material is p-type and must use a p-type absorbing layer. The unipolar barrier must be carefully engineered. It must be nearly lattice matched to the surrounding material and have a zero band offset in one band and a large offset in the other. If a suitable material cannot be found, a graded barrier can be created, but it can only be used as a minority carrier barrier; this graded barrier can only be used to block surface currents and minority currents. nBn and unipolar barrier devices in the InAs materials system have shown Auger limited performance comparable with the best HgCdTe detectors over a large temperature range, indicating the effectiveness of unipolar barriers when applied to infrared detectors.

C. Carbon Nanotube RF Transistors
   Investigator: Professor Peter Burke, UC Irvine, MURI
   Recipient: Carbonics

The objective of this research was to investigate carbon nanotube synthesis and understand their radio frequency (RF) properties for possible applications in RF electronics. To utilize the fundamental knowledge on manufacturing and testing carbon nanotube RF transistors developed in the PI's lab, Carbonics, a startup company specializing in carbon nanotube devices, hired the PI's student Dr. Rutherglen as its CTO. During his doctoral thesis research supported by the ARO MURI grant at UC Irvine, he published an authoritative review on nanoelectronic RF devices.[1] He also developed a comprehensive model to predict RF performance of nanotube transistors as a function of array pitch. He has transitioned carbon nanotube RF transistor technology developed in the PI's lab to Carbonics and continues to improve its performance. Recently at Carbonics, Dr. Rutherglen reported record performance of carbon nanotube RF transistors based on combined use of a self-aligned T-shape gate structure, and well-aligned, high-semiconducting-purity, high-density polyfluorene-sorted semiconducting

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[1] Rutherglen C, Jain D, Burke P. (2016). Nanotube Electronics for Radiofrequency Applications. *Nat. Nanotechnol.* 4: 811–819.

carbon nanotubes, which were deposited using dose-controlled, floating evaporative self-assembly method (see FIGURE 6). These transistors show outstanding direct current (DC) performance with on-current density of 350 µA/µm, transconductance as high as 310 µS/µm, and superior current saturation with normalized output resistance greater than 100 kΩ·µm. These transistors create a record as carbon nanotube RF transistors that demonstrate both the current-gain cutoff frequency (f t) and the maximum oscillation frequency (fmax) greater than 70 GHz. Furthermore, these transistors exhibit good linearity performance with 1 dB gain compression point (P1dB) of 14 dBm and input third-order intercept point (IIP 3) of 22 dBm. His study advances state-of-the-art of carbon nanotube RF electronics, which have the potential to be made flexible and may find broad applications for signal amplification, wireless communication, and wearable/flexible electronics.
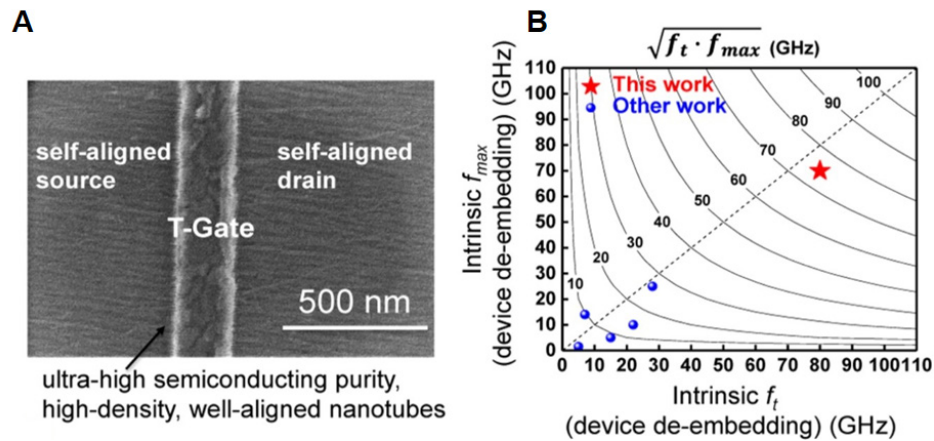

FIGURE 6

SEM image of aligned nanotubes for RF devices. (A) The cutoff frequency and fmax improve as per a formula described previously.[1] This work uses that formula for improved RF performance. Atomic Force Micrograph (AFM) of individual DNA Origami constructs. White scale bar = 100nm. (B) Cutoff frequency and maximum frequency of oscillation, using model developed by Rutherglen, for predicting and analyzing the performance of RF nano-devices. The record fMax achieved by Rutherglen using his PhD experience at UC Irvine applied in the context of startup Carbonics is shown.

D. Long Antenna Performance Achieved using Coupled Short Antenna Fragments
Investigator: Professor Kamal Sarabandi, University of Michigan, STIR Award
Recipient: ARL-SEDD, ARL-VTC, ONR

The goal of this research was to demonstrate that short antenna fragments can be electromagnetically coupled in the near field to result in antenna Q (quality factor), impedance, and bandwidth comparable to longer resonant antennas. Electrically short antennas, with lengths much shorter than a half-wavelength suffer from extremely high Q, low impedance, and very narrow bandwidth, in accordance with well-established theoretical grounds. Professor Sarabandi has demonstrated, for the first time, that electrically short antenna fragments can be coupled in the near field, with each driven by synchronized but separate power sources, resulting in lower Q, higher impedance, and wider bandwidth. So in a swarm of small, autonomous UAV's, where each UAV could only accommodate an small antenna, several UAV's could maneuver to emulate a larger resonant antenna. For example, an autonomous swarm of UAV's, operating well beyond line-of-sight of a controlling headquarters element, could emulate an HF antenna for reach-back communications or vehicles in a swarm of small UAV's operating in and around the buildings of an urban area could form an antenna for lower frequency communication or target detection penetrating the multiple building walls (see FIGURE 7).
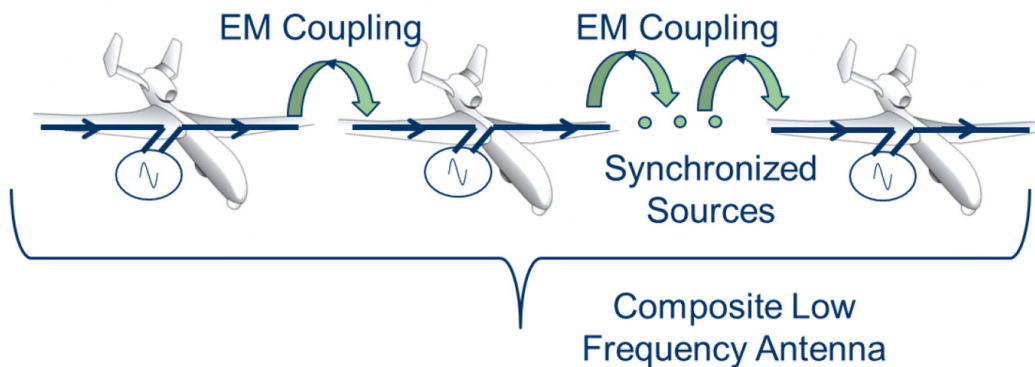
FIGURE 7

Concept for coupling electrically short antenna fragments. The three antenna elements of 1/10 wavelength were separated by a distance that varied between 1/10 and 1/20 wavelength. As the separation decreased (resulting in more coupling), the bandwidth and impedance varied from 10.6 MHz and 100 ohms, to 29 MHz and 200 Ohms, approaching the values for a single antenna, three times the length, 29 MHz and 250 Ohms.

The bandwidth and impedance were relatively insensitive to vertical movements of the antenna fragments (e.g., on UAVs), however they are very sensitive to lateral movements. Professor Sarabandi developed a technique to detect the lateral motion using optical sensors and compensate with an automatic matching control circuit (see FIGURE 8). He also developed a method to automatically synchronize the RF sources on the UAV's by coupling a master signal from the center UAV to negative resistance elements in the other UAV's (see FIGURE 9). These results were briefed to ARL-SEDD, ARL-VTD, ONR, Boeing, and ATD (AMRDEC). ARL-VTD initiated a collaboration for measurement for potential exploitation in the ARL MAST program. This research has transitioned to ONR, Boeing, and AMRDEC potential follow-on research.
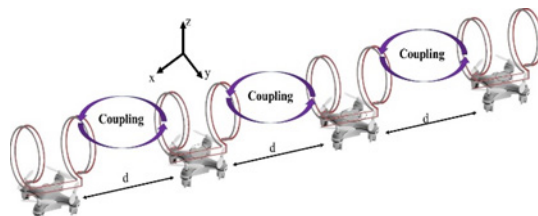

FIGURE 8

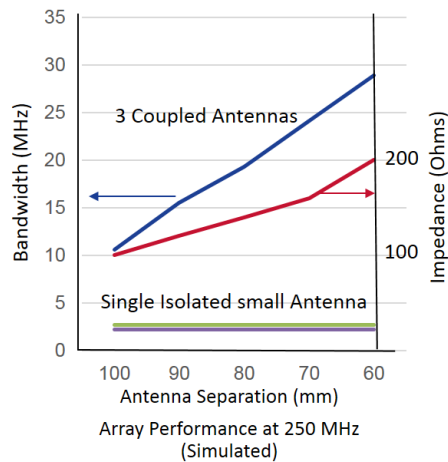Experimental setup of antenna configuration to explore bandwidth enhancement.

FIGURE 9

Dependence of bandwidth and impedance on antenna fragment separation. As the separation is varied from 1/10 wavelength to 1/20 wavelength, the bandwidth and impedance approach the values for a single resonant antenna 3 times as long (29 MHz and 250 Ohms).

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Vertical Transport in InAs/GaSb and InAs/InAsSb Superlattices
Professor Sanjay Krishna, University of New Mexico, STIR Award

The objective of this work is to determine the vertical and lateral transport properties of antimonide (Sb) based superlattices. Antimonide based superlattices have shown great potential for infrared imaging but still have not reached their theoretical limit. Much has been learned through various studies but a few important fundamental parameters are still unknown, key among them is the vertical mobility in this highly anisotropic system. In a superlattice vertical transport consists of moving through multiple interfaces and it is not clear whether making the interfaces sharper, as is norm in molecular beam epitaxy, will have a positive or negative impact on the transport (see FIGURE 10). Professor Krishna and other researchers from the Center for High Technology Materials at the University of New Mexico will collaborate with scientists from Air Force Research Laboratory, Naval Research Laboratory and the Sensors and Electron Devices Directorate at the Army Research Laboratory to perform a systematic theoretical and experimental program to investigate the vertical transport properties Type II Superlattices with initial emphasis on long wave Ga-free structures with Sb> 50%. The lateral and vertical mobilities and the minority carrier diffusion length in superlattices in the vertical direction will be determined using a scientific study comprising three parallel approaches using (i) magneto-transport measurements in high magnetic fields, (ii) pump-probe time of flight measurements, and (iii) EBIC (electron beam induced current) measurements. The results of the measurements will be compared and fed into a theoretical model for transport through layers. A close feedback loop between the theoretical effort and the experimental study will be implemented. The samples will be grown using molecular beam epitaxy and special care taken to isolate the effect of the conducting substrate from the electrical measurements. It is anticipated that in FY17 initial samples will be designed and grown and the measurements initiated. Each sample will be designed for the particular measurement being performed.
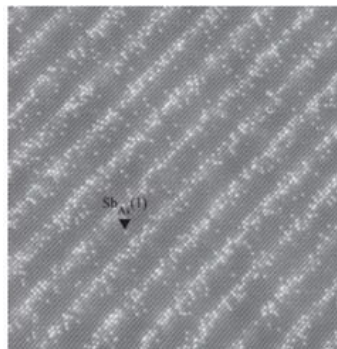

FIGURE 10

Anion images from a large-area Scanning Tunneling Microscopy (STM) survey of InAs/InAsSb superlattice.[2] The rough interfaces could promote carrier transport through the interfaces. Extremely smooth interfaces could localize holes in the InAsSb layer, thereby decreasing the vertical mobility. This research effort seeks to measure the vertical mobility and determine the limiting scattering mechanisms.

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[2] Wood MR, Kanedy K, Lopez F, Weimer M, Klem JF, Hawkins SD, Shaner EA, Kim JK. (2015). Monolayer-by-monolayer compositional analysis of InAs/InAsSb superlattices with cross-sectional STM. J. Cryst. Growth. 425: 110-114.

B. CMOS-enabled Massively-parallel Intracellular Nanowire Array
Professor Donhee Ham, Harvard University, Single Investigator Award

The goal of this project is to develop a high-density array of vertical nanowire electrodes on top of a CMOS integrated circuit (IC), to interface it with mammalian neuronal networks to record and stimulate neuronal signals in parallel and intracellular fashion, and to apply this unprecedented parallelization of intracellular interfacing for cellular-level neuroprosthetic operations on *in vitro* mammalian neuronal oscillators, blurring the biotic-abiotic boundaries in the hybrid bio-semiconductor systems. Building upon the experimental success with his first-generation chip (1,024 sites), the PI has fabricated a second-generation chip (4,096 sites) with much more improved circuit design and layout strategy. This newer chip has been successfully characterized electrically and electrochemically, demonstrating the sensitivity improvement by 10 times and is ready for electrophysiological experiments (see FIGURES 11-12).
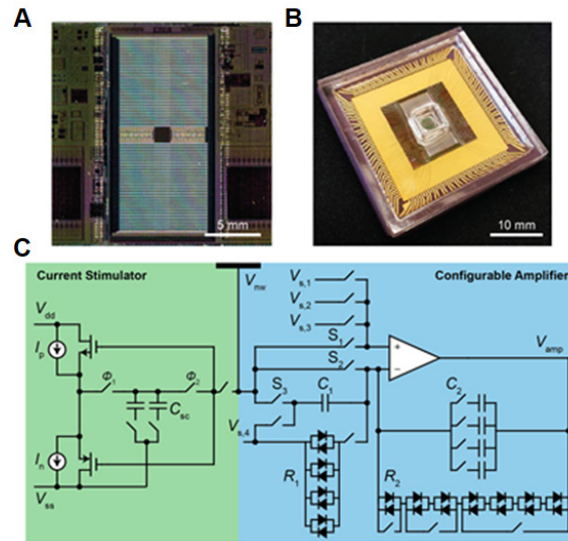

FIGURE 11

Second-generation chip (4,096 sites) with much more improved circuit design and layout strategy. (A) 2nd generation CMOS IC. (B) Packaged IC with nanoelectrodes post fabricated on top. (c) Simplified circuit schematic of pixel design; a current stimulator and configurable amplifier are implemented at each pixel to allow for various recording and stimulation modes.
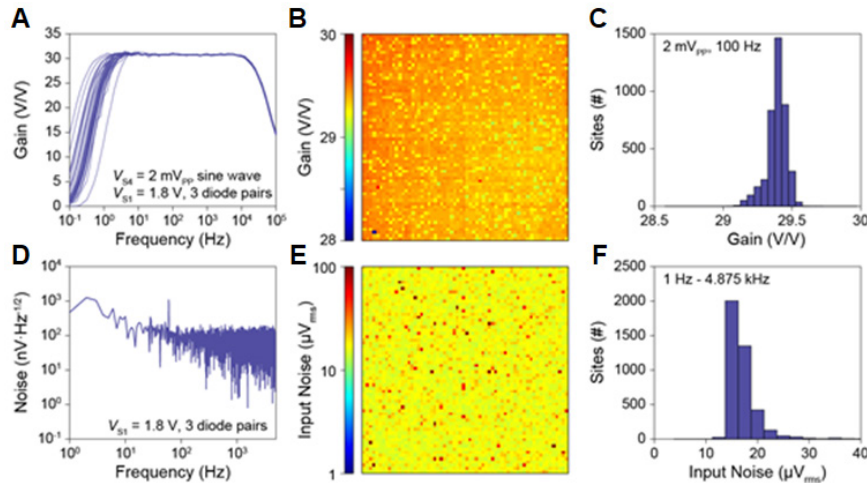

FIGURE 12

Performance of second-generation chip. (a) Measured transfer function of AC coupled configuration of the pixel amplifier in the second-generation chip. (b) Heat map of passband gain (Vamp/Vnw) at 100 Hz. (c)

Histogram of passband gain of (B). (**d**) Output voltage noise FFT of a typical amplifier. (**E**) Heat map of integrated Input referred noise from 1-4.875 kHz. (**F**) Histogram of integrated input referred noise of (**E**).

It is anticipated that in FY17 the research team will perform electrophysiological experiments with this second-generation chip by using both cardiomyocyte networks and neuronal networks, including neuronal oscillator networks. The immediate goal is to perform the parallel intracellular recording from both of these biological cellular networks. As compared to the work with the first-generation chip, the significant advance will be four fold. First, given the increased size of the array (from 1,024 sites to 4,096 sites), the research team expects to increase the number of sites where intracellular recording is performed simultaneously. Second, the 10 times improved sensitivity will facilitate the work with neuronal network (going beyond the cardiomyocyte tissue). Third, the new design of this chip, in particular, its stimulation current control, will further help improving the electroporation protocol, which is in particular important in treating the neurons. Fourth, this new chip with its improved design will allow more optimized manipulation of the network dynamics. It is also anticipated that the research team will in parallel develop third generation chip, where there is a closed-loop feedback between any site that is performing recording to any other sites to perform stimulation. While such closed-loop feedback can be performed off chip, it would lead too significant a latency to be practical. The on-chip closed feedback will facilitate the neuroprosthetic operation on the chip-scale platform.

C. Electro-optic Modulators with 2D Material based Microcavities
Professor Volker Sorger, George Washington University, Single Investigator Award

The objective of this research is to advance optical modulator high-speed and low energy/bit performance by investigating the incorporation of 2D materials into three microcavity regimes including microring, hybrid plasmonic and photonic crystal, and fully plasmonic. The three regimes will have a range of quality factors, insertion losses, areal footprints, and other factors that will influence the modulation depth and speed for a given driving voltage. Thermal management considerations will also be considered in terms of absorptive modulators. Potential focus of the work will in general be on EOMs (Electro-Optic Modulators) but the modulation physics could be either phase or amplitude modulation (see FIGURE 13). Research will be pursued in conjunction with ARL-SEDD thru a cooperative agreement. Results expected included efficient modulation at speeds up to 100 Gb/s, with efficiencies of around femtojoules/bit (orders of magnitude below many current approaches). The relevance of the optical modulators would be for Army battlefield communications, data processing, and related optical sensor and computational platforms. Particular potential is coming forth presently with the start of the DoD integrated photonics institute which this work could feed into in the long term. Advances in integrated photonics are being pursued primarily in silicon and indium phosphide material platforms, where graphene incorporation is already known to be possible. Other 2D materials may also be compatible but would need considered in terms of advanced processing in a high-throughput fashion. Nonetheless, the optical modulators show potential to advance both the speed and energy consumption metrics as well as reducing the areal footprint of such devices. The uses of such modulators is vast since optical switches are needed in almost every application of photonic integrated circuits. Ladar, sensors, data communications, and RF analog photonics are four major application areas identified already for such modulators.
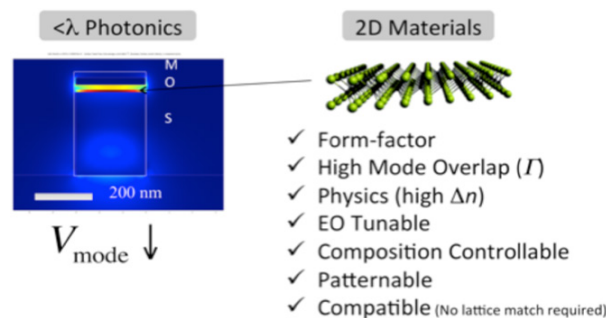

FIGURE 13
Proposed modulator scheme to incorporate 2D material active regions.

D. Coherent Phonon Beams for Communications and Spectroscopy
Professor Anthony Kent, University of Nottingham, Single Investigator Award (International Technology Center-Atlantic)

The objective of this research, co-funded through ARO and the RDECOM International Technology Center – Atlantic, is to explore new electronic functionality based on coherent phonons. Quantum well and superlattice structures will be pumped with coherent acoustic waves in order to acoustoelectrically generate THz frequency range electromagnetic waves. Sub-millimeter electromagnetic waves will be heterodyne mixed with THz acoustic waves in order to develop a new THz spectroscopy capability and applications to communications-on-a-chip functionality will be examined. It is anticipated that in FY17, high speed acousto-optical modulation of UV light will be demonstrated and explored as a means of manipulation of the light, and the team will develop new approaches to convert longitudinal-polarized bulk THz acoustic waves into transverse polarized bulk waves and surface waves, with potential application in acoustic spectroscopy, plasmonics, and optical modulation.
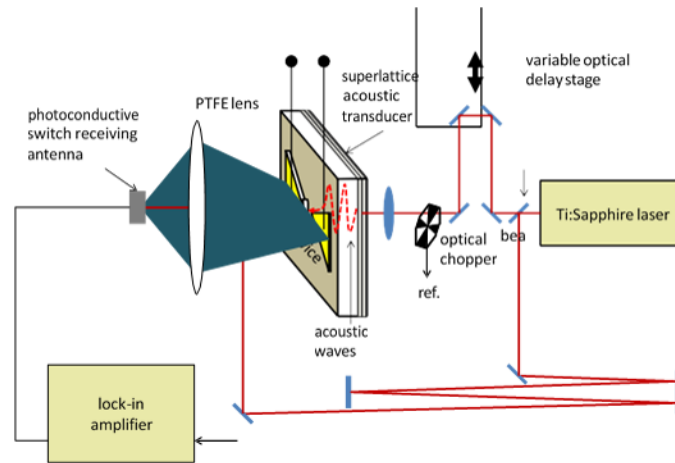

FIGURE 14

Experimental arrangement for measurement of the THz emission from straintronic devices. The long optical delay is to compensate for the time of flight of the acoustic waves across the device substrate.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. William Clark, III
Division Chief
Program Manager, Electronic Sensing

Dr. Michael Gerhold
Program Manager, Optoelectronics

Dr. James Harvey
Program Manager (Acting), Electromagnetics and Radio-frequency Electronics

Dr. Joe Qiu
Program Manager (Acting), Nano- and Bio-Electronics

B. Directorate Scientists

Dr. David Stepp
Director (Acting), Engineering Sciences Directorate

Dr. April Brown (IPA)
Research Scientist

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. LaToya Guidry
Administrative Specialist

Ms. Sade Sessoms
Contract Support

CHAPTER 6: LIFE SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2016* is to provide information on the programs and basic research supported by ARO in FY16, and ARO's mission to create basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Life Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and transitions facilitated by this Division in FY16.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Life Sciences Division supports research to discover and control the properties, principles, and mechanisms governing DNA, RNA, proteins, organelles, molecular and genetic systems, prokaryotic cells, eukaryotic cells, unicellular organisms, multicellular organisms, multi-species interactions, individual humans, and groups of humans. More specifically, the Division aims to promote basic research to elucidate the fundamental physiology underlying perception, cognition, neuro-motor output and non-invasive methods of monitoring cognitive states and processes during normal activity; basic research to understand antimicrobial resistance mechanisms; microbial community interactions including biofilm formation, cell-to-cell communications, population dynamics and host-pathogen/symbiont interactions; studies of organisms that are not culturable; studies of organisms at the single cell or mixed population (*e.g.*, metagenomic) level; studies of organisms that have adapted to grow or survive in extreme environments; identification and characterization of gene function, gene regulation, genetic interactions, gene pathways, gene expression patterns, mitochondrial regulation and biogenesis, nuclear and mitochondrial DNA replication, mutagenesis, oxidative stress, DNA repair, and regeneration; studies in structural biology, protein and nucleic acid structure-function relationships, molecular recognition, signal transduction, cell-cell communication, enzymology, cellular metabolism, and synthetic biology; and research to understand human behavior across different temporal, spatial and social scales. The results of this research will lay a foundation for future scientific breakthroughs and will enable new technologies and opportunities to maintain the technological and military superiority of the U.S. Army.

2. Potential Applications. Research managed by the Life Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the discoveries uncovered by ARO in the life sciences may provide new technologies for protecting the Soldier, for optimizing warfighter mental and physical performance capabilities, for creating new biomaterials, for advances in synthetic biology for energy production, intelligence, and bioengineering, and for new capabilities for predicting group behavior and change.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Life Sciences Division coordinates and leverages research within its Program Areas with many other agencies, including the Defense Threat Reduction Agency (DTRA), the Defense Advanced Research Projects Agency (DARPA), the Joint Improvised Explosive Device Defeat Organization (JIEDDO), the Army Natick Soldier Research Development and Engineering Center (NSRDEC), the U.S. Army Corps of Engineers (USACE), the Army Research Institute (ARI), the Army Medical Research and Materiel Command (MRMC), the Center for Disease Control (CDC), the National Institutes of Health (NIH), the Intelligence Advanced Research Projects Agency (IARPA), the Department of Homeland Security (DHS), the Army Criminal Investigation Laboratory (ACIL), the Federal Bureau of Investigation (FBI), the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AFOSR). In addition, the Division frequently coordinates with other ARO and ARL Divisions to co-

fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the ARO Chemical Sciences Division include promoting research to understand abiotic/biotic interfaces. The Life Sciences Division coordinates its research portfolio with the Materials Science Division to pursue the design and development of new biomaterials. The Life Sciences Division also coordinates extensively with the Mathematical Sciences Division to develop new programs in bioforensics, and with the Materials Science and the Mechanical Sciences Divisions to understand the effects of blast on synapses. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

In addition, the Division's research portfolio will reveal previously unexplored avenues for new Army capabilities while also providing results to support (i) the Human Sciences Campaign's goals to discover and predict human cognitive, physical, and social behaviors, as well as the role of training paradigms in building expertise, and to characterize the fundamental aspects of social network dynamics involving ethics, values, trust, social-cultural, economic, and geopolitical effects, (ii) the Assessment and Analysis Campaign's goal to identify human capabilities and limitations, (iii) the Information Sciences Campaign's goal to develop predictive models that consider the availability of power or food sources and the potential for social unrest or insurgency activity, (iv) the Sciences for Lethality-and-Protection Campaign's goal to predict and exploit interactions between information and humans, including the impact of trust and value on negotiation, and (v) the Materials Research Campaign's goal to exploit the evolutionary solutions created by nature and create similar structures using synthetic biology.

B. Program Areas

The Life Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY16, the Division managed research within these five Program Areas: (i) Genetics, (ii) Neurophysiology of Cognition, (iii) Biochemistry, (iv) Microbiology, and (v) Social and Behavioral Science. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Genetics. The scientific goals of this Program Area are to identify and characterize the mechanisms and factors that influence DNA stability and mutagenesis, gene expression, and genetic regulatory pathways in prokaryotes, eukaryotes, and eukaryotic organelles. This program also seeks to understand genetic instability at a population level. The program supports basic research on mitochondrial regulation and biogenesis, oxidative phosphorylation, oxidative stress, and the interactions and communication between the mitochondria and the nucleus. The Genetics Program also supports basic research to develop an empirical understanding of general mechanisms by which genomic, transcriptomic, and proteomic components respond to alterations in the population-genetic environment. A third area of emphasis is the identification, characterization, and modulation of genetic pathways and molecular cascades that determine the responses to stress and trauma. A final area of emphasis is to create the genetic foundation to be able to extract provenance information from both prokaryotic and eukaryotic DNA.

This Program Area supports high-risk, high payoff basic research that has the potential to create new Army capabilities, to optimize warfighter mental and physical performance capabilities, to reduce the effect of PTSD, stress, and pathogens on warfighter readiness and Army capabilities, and to develop new sources of intelligence.

2. Neurophysiology of Cognition. The objective of this Program Area is to support non-medically oriented research to elucidate the fundamental physiology underlying perception, sensorimotor integration and cognition. Examples of research areas under this program can include the psycho-physiological implications of brain-machine interfaces that optimize auditory, visual and/or somatosensory function; display and control systems based on physiological or psychological states; measuring and modeling individual cognitive dynamics and decision making during real-world activity and uncovering the cellular biology of neuronal function.

This Program Area is divided into two major research thrusts: (i) Multisensory Synthesis and (ii) Neuronal Computation. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. Research in the Multisensory Synthesis Thrust aims to understand how

the human brain functions in relation to the interaction of multisensory, cognitive and motor processes during the performance of real-world tasks. Basic research focused on mapping, quantifying and modeling distributed neural processes that mediate these features are being used to develop better understanding of the underlying bases of cognitive processes for eventual application to Soldier performance enhancement and improved human-machine symbiosis. Research in the Neuronal Computation Thrust is focused on understanding how living neuronal circuits generate desirable computations, affect how information is represented, show robustness to damage, incorporate learning and facilitate evolutionary change. Cell culture, brain slice and in vivo models are being used to develop better understanding of living neural networks for eventual application in Army systems that might include novel direct neural interfaces.

While these research efforts focus on high-risk, high pay-off concepts and potential long-term applications, current research may ultimately enable the development of neural biofeedback mechanisms to sharpen and differentiate brain states for possible direct brain-machine communication, identifying individual cognitive differences and new training paradigms for improved Soldier performance.

3. Biochemistry. The goal of this Program Area is to elucidate the mechanisms and forces underlying the function and structure of biological molecules. This research may enable the design and development of novel materials, molecular sensors and nanoscale machines that exploit the exceptional capabilities of biomolecules.

This Program Area supports two research Thrusts: (i) Biomolecular Specificity and Regulation, and (ii) Biomolecular Assembly and Organization. Within these Thrusts, innovative research efforts are identified and supported in pursuit of the vision of this program. Efforts in the Biomolecular Specificity and Regulation Thrust aim to identify the determinants of the specificity of molecular recognition and molecular activation/inactivation to modulate and control specificity and activity through protein engineering and synthetic biology approaches. Research in the Biomolecular Assembly and Organization Thrust aims to explore the fundamental principles governing biological self-assembly, to understand and control the relationships between molecular structure and biological material properties, and to identify innovative approaches to support biological activity outside of the cellular environment.

Research supported by this program promotes potential long-term applications for the Army that include biosensing platforms that incorporate the exquisite specificity of biomolecular recognition, nanoscale biomechanical devices powered by motor proteins, novel biotic/abiotic materials endowed with the unique functionality of biomolecules, drug delivery systems targeted by the activity and specificity of biomolecules, electronic and optical templates patterned at the nanoscale through biomolecular self-assembly, and novel power and energy systems that utilize biomolecular reaction cascades.

4. Microbiology. This Program Area supports basic research in fundamental microbiology. There are two primary research thrusts within this program: (i) Microbial Survival Mechanisms and (ii) Analysis and Engineering of Microbial Communities. The Microbial Survival Mechanisms thrust focuses on the study of the cellular and genetic mechanisms and responses that underlie microbial survival in the face of environmental stress. These stressors include extremes in temperature, pH, or salinity; the presence of toxins including metals and toxic organic molecules; oxidative stress; and cellular starvation and the depletion of specific nutrients. Research approaches include fundamental studies of microbial physiology and metabolism, cell biology, and molecular genetics that examine key cellular networks linked to survival, microbial cell membrane structure and the dissection of relevant critical signal transduction pathways and other sense-and-respond mechanisms. The Analysis and Engineering of Microbial Communities thrust supports basic research that addresses the fundamental principles that drive the formation, proliferation, sustenance and robustness of microbial communities through reductionist, systems-level, ecological and evolutionary approaches. Bottom-up analysis of information exchange, signaling interactions and structure-function relationships for single and multi-species communities within the context of planktonic and biofilm architectures is considered. Of joint interest with the ARO Biomathematics Program, research efforts that advance our ability to work with complex biological data sets to increase understanding of microbiological systems marked by ever-increasing complexity are considered.

While these research efforts focus on high-risk concepts, research supported by this program promotes a range of long-term applications for the Army, including strategies for detecting and classifying microbes, for controlling bacterial infections, for harnessing microbes to produce novel materials, to protect materiel, and/or to efficiently produce desirable commodities. In addition, understanding how microbes adapt is crucial for advancing studies in other fields, including genetics, environmental science, materials science, and medicine.

5. Social and Behavioral Science. The goal of this Program Area is to gain a better theoretical understanding of human behavior at all levels, from individuals to whole societies, for all temporal and spatial scales, through the development of mathematical, computational, simulation and other models that provide fundamental insights into factors contributing to human socio-cultural dynamics and societal outcomes (see FIGURE 1).

This Program Area is divided into two research Thrusts: (i) Predicting Human Social Behavior, and (ii) Complex Human Social Systems. The program supports research that focuses on the theoretical foundations of human behavior at various levels (individual actors to whole societies) and across various temporal and spatial scales. This includes, but is not limited to, research on the evolution and dynamics of social systems and organizations, human adaptation and response to both natural and human induced perturbations (*e.g.*, global climate change, mass migration, war, attempts at democratization, movements for social justice), interactions between human and natural systems, the role of culture and cognition in accounting for variations in human behavior, human decision-making under risk and uncertainty, the search for organizing principles in social systems, and the emergent and latent properties of dynamic social systems and networks. The research involves a wide range of approaches, including computational modeling, mathematical modeling, agent-based simulations, econometric modeling and statistical modeling, comparative-historical analyses, to name a few. The program also recognizes the fact that the building and validation of models in the social sciences is often limited by the availability of adequate and appropriate sources of primary data. A component of supported research includes the collection of primary data for model development and testing. The program also supports research to develop methodologies (*e.g.*, measurement, data collection, statistical methods, and research designs) that may provide an improved scientific understanding of human behavior.
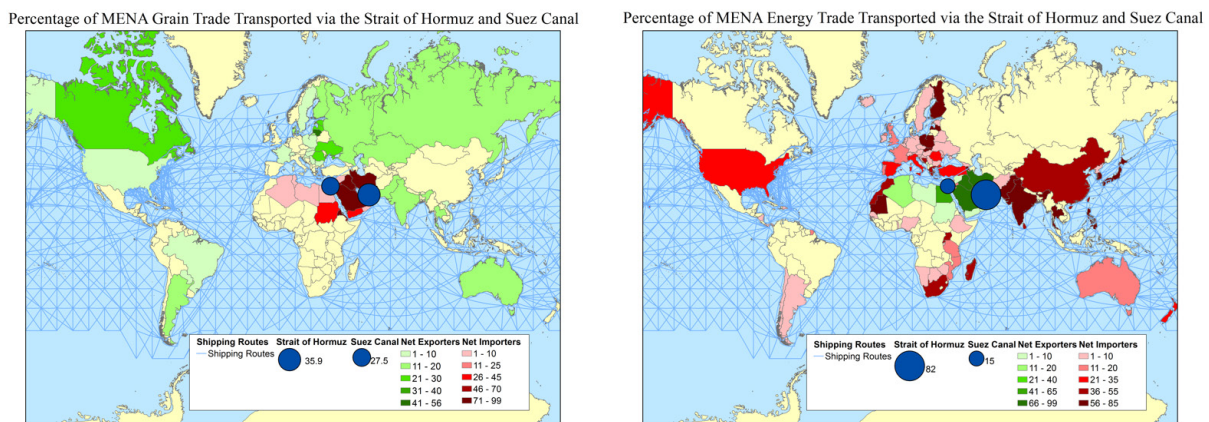

FIGURE 1

Estimates of shipping transportation routes for exporters and importers of fuel and grain trade to Middle East and Northern Africa regions. This research shows the comprehensive trade systems and routes through which grain (left panel) is imported to MENA and fuel is exported from MENA . As the map indicates, the Strait of Hormuz and Suez Canal represent major choke points signified by large blue circles, which if compromised, could generate considerable conflict and instability across the region. This is especially the case for countries with dark red shading, where as much as 99% of grain imports flow through these routes. In addition, exporters would suffer a constraint on fuel imports, further compromising grain exports, increasing the likelihood of conflict and sociopolitical instability in MENA states, which are already volatile. This demonstrates the complex interrelationships between trade across different domains and sociopolitical dynamics on a global scale.

Research focuses on high-risk approaches involving highly complex scientific problems in the social sciences. Despite these risks, the research has the potential to make significant contributions to the Army through applications that will, for example, improve decision-making at various levels (policy, combat operations), create real-time computer based cultural situational awareness systems for tactical decision-making, increase the predictability of adversarial and allied intent, and produce integrated data and modeling in situ for rapid socio-cultural assessment in conflict zones and in humanitarian efforts.

C. Research Investment

The total funds managed by the ARO Life Sciences Division for FY16 were $128.7 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY16 ARO Core (BH57) program funding allotment for this Division was $7.7 million and $1.0 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $10.8 million to projects managed by the Division. The Division also managed $86.4 million of Defense Advanced Research Projects Agency (DARPA) programs, $2.9 million for Minerva Research Initiative projects, and $1.6 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.9 million for contracts. The Army's Institute for Collaborative Biotechnologies received $11.0 million. Finally, $5.6 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which included $0.2 million of the Division's total ARO Core (BH57) funds, in addition to funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY16 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY16 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY16, the Division awarded 26 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Victor Asal, State University of New York (SUNY) at Albany; *The Organization that Does(n't) Bark: Organizations and the Decision for Political Violence*
- Professor Antoni Barrientos, University of Miami School of Medicine; *Mitochondrial Regulation of Neurodegenerative Proteotoxic Stress*
- Professor Ross Carlson, Montana State University; *Development of Robust Microbial Communities through Engineered Biofilms*
- Professor Jose Carmena, University of California - Berkeley; *High-speed Volumetric Two-Photon Microscope for the Study of Neural Circuits*
- Professor Amit Choudhary, Brigham and Women's Hospital; *Chemical Countermeasures for CRISPR-Cas9/Cpf1 enzymes*
- Professor Bryan Davies, University of Texas - Austin; *Dessication-induced Persistence*
- Professor Melik Demirel, Pennsylvania State University; *Revolutionary Properties of Evolutionary Biological Materials*
- Professor Danielle Ercek, Northwestern University Evanston Campus; *Engineering Nanoscale Protein Containers*
- Professor John Evans, New York University; *Sea Urchin Spicules: Assembly Of Fracture-Toughened Materials At The Nano- And Meso-Scale*
- Professor Stephen Fuchs, Tufts University; Identification and evolution of adhesive peptides with novel specificity using yeast surface display
- Professor Robert Kuchta, University of Colorado - Boulder; *Redox Responsive Dynamic DNA Nanomaterials*
- Professor Philip Lukeman, St. John's University, New York; *A Polyvalent, Allosteric Whole-Virus Binding Platform for Norovirus Detection*

- Professor E. Neil Marsh, University of Michigan - Ann Arbor; *A Flexible Symmetry-Based Approach to Assembling Protein Nano-Cages*

- Professor Dan Mishmar, Ben Gurion University of the Negev; *Exploring The Regulatory Cross Talk Between The Mitochondrial Genetic System And Stressful Physiological Conditions In The Battlefield*

- Professor Stephen Mitroff, George Washington University; *Examining Learning And Influences On Performance In Visual Search*

- Professor Yuan Pang, Mayo Clinic   *Genetic and Structural Approach to Disease-Vector Control to Protect US Troops against Leishmaniasis and Malaria*

- Professor Sumita Pennathur, University of California - Santa Barbara; *Extending the Mechanisms of Protein Function to Non-Cellular Environments*

- Professor Alan Poling, Western Michigan University; *Improving Performance of Landmine-Detection Rats*

- Professor William Reed, University of Maryland - College Park; *Biophysiological and Social Predictors of Political Violence*

- Professor Jasper Rine, University of California - Berkeley; *Actionable Variation in Human Genes to Enhance Metabolic Efficiency*

- Professor Paul Sajda, Columbia University; *Intent Switching and Co-Adaption of Man and Machine in a Closed-Loop Brain Computer Interface*

- Professor Daniel Schwartz, University of Colorado - Boulder; *Single Molecule Resolution Of Peptide-Lipopolysaccharide Interactions*

- Professor Peter Setlow, University of Connecticut - Health Center; *Metabolic Activities in Dormant Spores of Bacillus Species*

- Professor Boleslaw Szymanski, Rensselaer Polytechnic Institute; *Forecasting Emergent Phenomena with Human Computer Collaboration*

- Professor Cedric Williams, University of Virginia; *Facilitation of Olfactory Discrimination & Generalization Learning*

- Professor Cheng Zhu, Georgia Tech Research Corporation; *Mechanical Regulation Of Integrin Conformation*

2. Short Term Innovative Research (STIR) Program. In FY16, the Division awarded four new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Julie Biteen, University of Michigan - Ann Arbor; *Capturing The Dynamic Response Of Microbes To Their Environment And Their Community*

- Professor William Doolittle, Georgia Tech Research Corporation; *Biologically Realistic Ionic Retina*

- Professor Edward Keefer, Nerves Incorporated; *The Molecular And Electrophysiologic Response To Chronic Intraneural Silicone Electrode Implantation*

- Professor Lei Li, University of Notre Dame; *Melatonin Modulation Of The Olfacto-Retinal Centrifugal Visual Pathway*

- Professor Ramin Pashaie, University of Wisconsin - Milwaukee; *Multi-Modal Brain Interface System for the Study of Neurovascular Coupling*

3. Young Investigator Program (YIP). No new starts in this category were awarded in FY16.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY16 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *The Influence of States and Traits on Individual and Group Performance Variability*; Baltimore, MD; 24-25 March 2016

- *Symposium SM9 on Structure and Properties of Biological Materials and Bioinspired Designs* (part of 2016 Spring Materials Research Society Meeting); Phoenix, AZ; 28 March - 1 April 2016

- *13th Conference on the Foundations of Nanoscience (FNANO 2016)*; Snowbird, UT; 11-14 April 2016
- *Gordon Research Conference on Biointerface Science*; Les Diablerets, Switzerland; 11-17 June 2016
- *Microbial Stress Response Gordon Research Conference*; South Hadley, MA; 17-22 July 2016
- *FASEB Science Research Conference on Virus Structure and Assembly*; Steamboat Springs, CO; 24-29 July 2016
- *Cross-Cultural Decision Making to Advance Understanding of Human Aspects of the Operational Environment*; Orlando, FL; 29 July 2016

5. Special Programs. In FY16, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded ten new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Blast Induced Thresholds for Neuronal Networks. This MURI began in FY10 and was awarded to a team led by Professor David Meaney at the University of Pennsylvania. This research is jointly managed with the ARO Mechanical Sciences Division. The objective of this MURI is to understand the effects of a primary blast wave and how it can cause persistent damage to the nervous system and the brain at the meso- and micro-scale.

The research team will build and validate a model of the human brain/skull subject to blast loading and use this model to scale blast field conditions into cell culture and animal models. This research will develop multiscale blast thresholds for alteration of synapses, neuronal connectivity, and neural circuits (*in vitro* and *in vivo*) and will examine if these thresholds change for tissue and/or circuits in the blast penumbra. Finally, the researchers will determine the blast conditions necessary to cause persisting change in neural circuitry components (up to two weeks) and will correlate alterations in circuits to neurobehavioral changes following blast. This research should provide a basis for shifting defensive armor design efforts from defeating the threat based on material deformation, damage, and rupture, to mitigating the effects based on biological relevance. In addition the research may lead to medical applications for treating neurotrauma and in regenerative medicine.

2. Prokaryotic Genomic Instability. This MURI began in FY10 and was awarded to a team led by Professor Patricia Foster at Indiana University. The objective of this research is to identify and extract the mathematical signatures of prokaryotic activity in DNA.

The investigators are characterizing fundamental parameters in the microbial mutation process in a superior model system, including both cell-mechanistic and evolutionary components. The research is a comprehensive effort with strong experimental and computational components. The team will determine the contribution of DNA repair pathways, cellular stress, and growth conditions on the mutation rate and mutational spectrum of *E. coli* using whole genome sequencing over the course of strain evolution. The team is extending this analysis to a panel of twenty additional eubacterial species. To understand the forces that define short-term and long-term evolutionary mutation patterns, a new class of population-genetic models will also be developed. The investigators will include mutant strains with known deficiencies in genome maintenance. Parallel analyses in such strains will produce larger data sets that define, by comparison to wild type strains, the contribution of each repair pathway to the overall mutational spectrum. Mutational changes characteristic to specific environmental conditions/stresses/genotoxicants can be analyzed in the context of the mutational signatures of individual repair pathway throughout the genome. Overall, the proposed research presents an unprecedented opportunity to uncover patterns of mutational variation among prokaryotes. The approach is unique in that the investigators are using a comprehensive whole-genome, systems-biology approach to characterize and understand DNA instability at a whole-genome level, across a comprehensive range of prokaryotes.

3. Translating Biochemical Pathways to Non-Cellular Environment. This MURI began in FY12 and was awarded to a team led by Professor Hao Yan at Arizona State University. This MURI is exploring how biochemical pathways could potentially function in a non-cellular environment.

Cells provide a precisely organized environment to promote maximum efficiency of biochemical reaction pathways, with individual enzymatic components organized via multisubunit complexes, targeted localization in membranes, or specific interactions with scaffold proteins. The eventual translation of these complex pathways to engineered systems will require the ability to control and organize the individual components outside of the natural cellular environment. Although biological molecules have been successfully attached to inorganic materials, this process often requires chemical modification of the molecule and can restrict its conformational freedom. An alternative approach to maintain biological activity outside of the cell, while preserving conformational freedom, is to encapsulate enzymes within specialized materials or structures. Unfortunately, surface patterning of current encapsulating agents has not achieved the precision required to replicate the organizational capabilities of the cell.

The objective of this research is to develop the scientific foundations needed to design, assemble, and analyze biochemical pathways translated to a non-cellular environment using 3D DNA nanostructures. The MURI team is using DNA nanostructures to direct the assembly of selected biochemical pathways in non-cellular environments. The focus of this research is to develop the scientific foundations needed to translate multi-enzyme biochemical reaction pathways from the cellular environment to non-biological materials. The ability to translate biochemical reaction pathways to non-cellular environments is critical for the successful implementation of these pathways in DoD-relevant technologies including responsive material systems, solar cells, sensor technologies, and biomanufacturing processes.

4. Evolution of Cultural Norms and Dynamics of Socio-Political Change. This MURI began in FY12 and was awarded to a team led by Professor Ali Jadbabaie at the University of Pennsylvania. This MURI is exploring the cultural and behavioral effects on societal stability.

Recent events involving the diffusion of socio-political change across a broad range of North African and Middle Eastern countries emphasize the critically important role of social, economic and cultural forces that ultimately affect the evolution of socio-political processes and outcomes. These examples clearly demonstrate that radically different outcomes and chances for conditions of state stability result from the different institutional frameworks within these countries. It is well established in the social sciences that change in or evolution of institutions depends on the behavior patterns or culture of the people involved in them, while these behavior patterns depend in part on the institutional framework in which they are embedded. This dynamic interdependence of culture and institutional change means that the modeling of societal stability requires the coupling of individual modeling approaches describing such issues as trust and cooperation with models describing institutional dynamics.

The objective of this MURI is to develop fundamental theoretical and modeling approaches to describe the complex interrelation of culture and institutions as they affect societal stability. The research team is extending the cultural approaches from application to individuals, families, and villages, to address stability of the larger social group. The models developed in this MURI may ultimately provide guidance in data collection and analysis of data on local populations that can provide planners with models to anticipate the second or third-order ramifications of actions that impact local populations.

5. Simultaneous Multi-synaptic Imaging of the Interneuron. This MURI began in FY12 and was awarded to a team led by Professor Rafael Yuste at Columbia University. The research team is exploring how individual neurons act as computational elements.

Interneurons are highly networked cells with multiple inputs and outputs. It has been to date impossible to record all the inputs and outputs from even a single living interneuron with synaptic levels of resolution in a living brain. While there is information on the morphological, physiological, and molecular properties of interneurons as a class and on their general synaptic connections, there is still little direct information on the functional roles of individual interneurons in cortical computations, and especially not on how each synapse relates to all the others within a single cell. Coupled with tagging via fluorescent molecules and/or chromophores and genomic modifications to control co-expression, electro-optical imaging may provide a solution, due to its ability to achieve subwavelength resolution across a relatively wide field of view.

The objective of this research is to explain and quantitatively model the entire set of neurotransmitter flows across each and every individual synapse in a single living interneuron, with experimental preparations ranging from cell culture systems through model neural systems. The research team will use genetically-engineered mice expressing specific labels in specific interneurons, high-throughput electron microscopy, and super-resolution imaging techniques to reveal the connectivity and the location of the synapses. This research may ultimately provide models that predict the information transitions and transformations that underlie cognition at the smallest scale where such activity could take place. These models could revolutionize the understanding of how human brains instantiate thought, and may lead to applications such as neural prostheses.

6. Artificial Cells for Novel Synthetic Biology Chassis. This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj at the University of California - San Diego. The goal of this MURI is to understand how biological and biomimetic synthetic cellular elements can be integrated to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways. This research is co-managed by the Life Sciences and Chemical Sciences Divisions.

The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as chassis for the engineered biological systems and devices. While single-celled organisms (e.g., bacteria, yeast) are typically used as synthetic biology chassis, the complexity of even these relatively simple organisms presents significant challenges for achieving robust and predictable engineered systems. A potential solution is the development of minimal cells which contain only those genes and biomolecular machinery necessary for basic life. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, and composite microparticles with stable internal compartments. These advances provide the scientific opportunity to explore the integration of biological and biomimetic elements to generate an artificial hybrid cell that for the first time combines the specificity and complexity of biology with the stability and control of synthetic chemistry.

The objective of this MURI is to integrate artificial bioorthogonal membranes with biological elements to create hybrid artificial cells capable of mimicking the form and function of natural cells but with improved control, stability, and simplicity. If successful, these artificial cells will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology that may ultimately enable sense-and-respond systems, drug-delivery platforms, and the cost-effective production of high-value molecules that are toxic to living cells (e.g., alternative fuels, antimicrobial agents).

7. Force-activated Synthetic Biology. This MURI began in FY14 and was awarded to a team led by Professor Margaret Gardel at the University of Chicago. The goal of this MURI is to understand the mechanisms by which biochemical activity is regulated with mechanical force and reproduce the mechanisms in virtual and synthetic materials. This research is co-managed with the Materials Science Division.

A critical aspect of synthetic biology systems is the targeted and controlled activation of molecules affecting biological function. Molecules can be activated by a variety of different signals, including chemical, optical and electrical stimuli, and synthetic biological circuits responsive to each of these stimuli have been successfully assembled. In recent years, the ability of mechanical force to serve as a biological signal has emerged as a unique and unexpected facet to biological activation. The rapidly growing field of mechanotransduction is beginning to reveal an extraordinary diversity of mechanisms by which mechanical forces are converted into biological activity. This field has been heavily influenced and driven through ARO-funded research, including a prior MURI.[1] Despite these rapid advances, mechanophores have never been incorporated into advanced synthetic material. This research area provides an exceptional opportunity to integrate biological activation by

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[1] Potisek SL, Davis DA, Sottos NR, White SR, Moore JS. (2007). Mechanophore-linked addition polymers. *J Am Chem Soc*.129:13808-9.

Davis DA, Hamilton A, Yang J, Cremar LD, Van Gough D, Potisek SL, Ong MT, Braun PV, Martínez TJ, White SR, Moore JS, Sottos NR. (2009). Force-induced activation of covalent bonds in mechanoresponsive polymeric materials. *Nature*. 459:68-72.

Lenhardt JM, Ong MT, Choe R, Evenhuis CR, Martinez TJ, Craig SL. (2010). Trapping a diradical transition state by mechanochemical polymer extension. *Science*. 329:1057-60.

Burnworth M, Tang L, Kumpfer JR, Duncan AJ, Beyer FL, Fiore GL, Rowan SJ, Weder C. (2011). Optically healable supramolecular polymers. *Nature*. 472:334-7.

mechanical force into the growing toolbox of synthetic biology, and to establish unprecedented paradigms for the incorporation of highly specific force activation and response into new materials.

The objective of this research is to elucidate the molecular mechanisms by which living cells regulate intracellular biochemical activity with mechanical force, to reproduce and analyze these force-activated phenomena in synthetic and virtual materials, and to design and exploit optimized synthetic pathways with force-activated control. If successful, this research may dramatically influence future advances in engineered biological systems, materials synthesis and fabrication, and force-responsive and adaptive bio-mimetic material systems.

8. Innovation in Prokaryotic Evolution. This MURI began in FY14 and was awarded to a team led by Professor Michael Lynch at Indiana University - Bloomington. The goal of this MURI is to model evolution in nutrient-deprived bacterial cultures, and then characterize changes in the genetic, metabolic, and social networks to create models that reflect the complexities of group evolution.

Classical Darwinian evolution selects for individuals that are better than others of their species in critical areas associated with reproductive fitness. For example, giraffes are selected for longer necks and cheetahs are selected for running speed. Similarly, single-celled organisms growing in rich media are selected for their ability to reproduce more quickly. In contrast, organisms that have run out of food can no longer simply improve at what they are already able to do; they are forced to innovate new methods to exploit previously untapped resources. In times of scarcity, even unicellular organisms rapidly evolve into complex societies with assorted subpopulations formed with unique and specialized skills. It is no longer an effective strategy to grow faster during starvation. In short, evolution during lean times requires the group to evolve as a whole, as each individual competes, cooperates, and depends on other members of the group.

The objective of this research is to develop a model of evolution in isolated independent cultures of organisms that are starving for months or years, and then model change in the genetic, epigenetic, transcriptomic, proteomic, metabolomic, and social networks to create experimentally-validated, mathematically-rigorous, and predictive models that accurately reflect the real complexities of group evolution. In the long term, the results of this research may lead to new applications for safer, economical food and water storage, new mechanisms to control and kill pathogens that will impact wound healing, diabetes, heart disease, dental disease, and gastrointestinal disease.

9. Imaging and Control of Biological Transduction using Nitrogen Vacancy Diamond. This MURI began in FY16 and was awarded to a team led by Professor Ronald Walsworth at Harvard University. The goal of this MURI is to further develop nitrogen vacancy nanodiamonds as non-biological quantum sensors and engineer a biological interface for actuating biological processes. This research is co-managed with the Physics Division.

The nitrogen vacancy center lattice defect in diamond nanoparticles (NV-diamond) can retain activity in biological environments. Current applications of NV-diamond include quantum computing, nanoscale magnetometry, super-resolution imaging and atomic scale magnetic resonance imaging. These state of the art applications involve NV-diamonds implanted in substrates; however recent breakthroughs have allowed isolated nano-diamond particles to be used as biosensing intracellular quantum probes for thermometry and bacterial tracking as well as extracellular quantum probes of ion channel operation. A key reason for NV-diamond sensitivity, including in the emerging biosensing applications, is that the spectral shape and intensity of optical signals from NV-diamond are sensitive to external perturbation by strain, temperature, electric fields and magnetic fields. Biological sensory transduction relies upon highly evolved ion channel-based mechanisms that involve transducing environmental energy into a bioelectrical signal for intercellular communication. The recent demonstrations of NV-diamond's extreme sensitivity and localization now provide new research opportunities for transitioning NV-diamonds from passive sensors to novel biophysical interfaces whose perturbed energy emission can be used as a signal to control or modify sensory transducer molecular physiology and intra- and inter-cellular signaling.

This multidisciplinary project four closely-coupled aims: (1) to optimize nitrogen vacancy nanodiamond synthesis, (2) to realize stable, biocompatible nanodiamond surface functionalizations, (3) to advance nitrogen vacancy sensitivity to chemical and biological systems and (4) to enable nitrogen vacancy-based manipulation of biological transduction. Systematically studying the integration of nitrogen vacancy nanodiamonds with reconstituted or native ion channels will lead to greater understanding but will, more importantly, create a new

paradigm for exogenous control of biological transduction events and the ability to uncover fundamental mechanisms with unprecedented spatial and temporal resolution. The outcome from this endeavor will lead to significant scientific breakthroughs in understanding how to develop and control quantum systems capable of interfacing with, and controlling, biological systems. If successful, the research efforts may improve future Army capabilities ranging from advanced artificial intelligence systems, early diagnosis and effective treatment of neurological disorders at the cellular and network levels, novel human-machine interfaces, and antidotes to neurotoxins, pathogens, and other diseases.

10. Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery. This MURI began in FY16 and was awarded to a team led by Professor Michael Jewett at Northwestern University – Evanston. The goal of this MURI is to engineer the translation machinery to accept and polymerize non-biological monomers in a sequence-defined manner using non-traditional chain growth polycondensation chemistries (beyond amide and ester linkages). This research is co-managed by the Chemical Sciences (lead) and Life Sciences Divisions.

Employing only four nucleotides and twenty amino acids, a plethora of biopolymers (e.g., proteins, DNA) with precisely-defined building block sequence gives these materials the ability to fold into higher-ordered structures capable of performing a variety of advanced functions such as information storage, self-replication, and signal transduction. The ability to extend comparable molecular-level sequence control to synthetic polymers, which have a much wider range of monomeric building blocks, has many scientific and technological implications, as it would enable precise control over structure-property relationships. Recent work has demonstrated that altering the sequence of short conjugated phenylene-vinylene oligomers can significantly modulate both electronic and optical properties. While greater complexity in function is anticipated for longer chain sequence-defined polymers, chemical routes to their synthesis have remained elusive. Conversely, biology synthesizes long sequence-defined polymers with extremely high efficiency and accuracy by employing templates to provide sequence information. More specifically, the ribosome, the workhorse of the translation machinery, is very adept at sequence-defined polymer synthesis through the successive condensation of amino acids (monomers), but primarily performs a single type of chemistry—amide bond formation via a chain-growth condensation polymerization. Co-opting the natural translation machinery to accept non-biological monomers is an attractive approach to synthesize non-biological polymers with the sequence control of biology. However, this approach is limited by cell viability constraints; thus, in vitro engineering of the translation machinery may offer unprecedented freedom of design to modify and control ribosome chemistry.

The objective of this research is to engineer and repurpose the translation apparatus (including the ribosome and the associated factors needed for polymerization) to produce new classes of sequence-defined polymers. In the long term, this research may enable a broad range of disruptive technologies having significant impact on DoD capabilities. Sequence control at the atomic level will give the greatest possible control over the emergent, macroscopic behavior of oligomers and polymers, leading to new advanced personal protective gear, sophisticated electronics, fuel cells, advanced solar cells, and nanofabrication, which are all key to the protection and performance of soldiers.

11. Defining Expertise by Discovering the Underlying Neural Mechanisms of Skill Learning. This MURI began in FY16 and was awarded to a team led by Professor Scott Grafton at the University of California – Santa Barbara. The goal of this MURI is to Uncover the temporal dynamics of neural substrates and cognitive processes engaged during skill learning and generate a definition of expertise based on the underlying neurocognitive computational advantages generated through learning. This research is co-managed by the Life Sciences (lead) and Mathematical Sciences Divisions.

Neuroscience, social psychology and education are providing insights into neural and cognitive processes involved during skill learning which show structural and functional differences in multiple brain regions when compared between 'experts' and 'novices'. Typically, these comparisons involved a novice time point and an expert time point because of the difficulty measuring intracranial brain activity over the course of skill learning. Novel materials now enable long-term implantation of high density neural recording devices in humans and animal models. Emerging engineering breakthroughs enable spike and local field potential recording from multiple neuroanatomical sites in the brain simultaneously. However, a major analytical barrier prevents easily linking this high density data with data acquired through existing non-invasive electrophysiology techniques and other tools for determining structure-function relationships like magnetic resonance imaging.

The objective of this research is to develop tools and techniques that can both predict and explain from a neurobiological perspective, why there are differences among individuals in their ability to develop expertise. The future force demands expert soldier performance across many tasks. In the long term, this basic research effort will provide a critical foundation for developing training methods based on computational and network neuroscience that are grounded in neurophysiology and neuroanatomy.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY16, the Division managed two new-start SBIR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY16 and a list of prior-year topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY16, the Division managed three new-start STTR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of STTR topics published in FY16 and a list of prior-year topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY16, the Division managed two new ARO (Core) HBCU/MI projects and six new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The following PECASE recipient, previously nominated by this Division, was announced in this fiscal year by the White House. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Governmentality and Social Capital in Tribal/Federal Relations Regarding Heritage Consultation. The objective of this PECASE, led by Professor Sarah Cowie at the University of Nevada - Reno, is to develop a model for improved heritage consultation between the federal government and tribal leaders based on a new theoretical approach to social relationships.

This research effort involves a qualitative study of the impasse in federal/tribal discourses regarding heritage consultation, and collaboratively develop a model for improved consultation procedures. The study will address the repercussions of federal government discourse surrounding indigenous heritage and the utility of social capital for improving communication. The proposed model and strategies under this effort can lead to long-term, productive relationships for improved preemptive heritage consultation. This would also provide a shift in current discourse towards future relationships between the Army and local populations in other countries.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY16, the Division managed nine new

DURIP projects, totaling $1.8 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. University Affiliated Research Center (UARC): Army Institute for Collaborative Biotechnologies (AICB)

The AICB is managed by ARO on behalf of the Army and is located at the University of California, Santa Barbara (UCSB), in partnership with the Massachusetts Institute of Technology (MIT), the California Institute of Technology (Caltech) and industry. The scientific objective of the AICB is to investigate the fundamental mechanisms underlying the high performance and efficiency of biological systems and to translate these principles to engineered systems for Army needs. Through research and strategic collaborations and alliances with Army laboratories, Research, Development and Engineering Centers (RDECs), and industrial partners, the AICB provides the Army with a single conduit for developing, assessing and adapting new products and biotechnologies for revolutionary advances in the fields of biologically-inspired detection, materials synthesis, energy generation and storage, energy-dispersive materials, information processing, network analysis and neuroscience. A total of $11 million was allocated to the AICB in FY16, which was the third year of the contract that was amended in FY14 for the next five-year period. Of these FY16 funds, $7.5 million was allocated for 6.1 basic research and $1.2 million was allocated for four 6.2 projects.

In FY16, the AICB supported 39 faculty members, 78 graduate students, and 50 postdoctoral fellows across 13 departments at UCSB, Caltech and MIT. The research falls into six Thrusts: (i) Systems and Synthetic Biology, (ii) Control and Dynamical Systems, (iii) Photonic and Electronic Materials, (iv) Cellular Structural Materials, (v) Biotechnology Tools, and (vi) Cognitive Neuroscience. Detailed descriptions of each core research Thrust and corresponding projects are available at the AICB program website (*http://www.icb.ucsb.edu/research*). A U.S. Army Technical Assessment Board and an Executive Steering Board biennially review the AICB research portfolio, assessing the project goals and accomplishments and set goals for the coming year.

I. DARPA Systems-Based Neurotechnology for Emerging Therapies (SUBNETS) Program

The goal of this program is to create an implanted, closed-loop diagnostic and therapeutic system for treating, and possibly even curing, neuropsychological illness in humans. ARO Life Sciences co-manages SUBNETS projects focused on treatments to restore normal functionality following injury to the brain or the onset of neuropsychological illness. The major approach supported through this program involves clinical trials which will use current FDA-approved implantable intracranial recording devices in neurosurgical patients with psychiatric, epilepsy, movement disorder, and pain conditions in order to identify the corresponding 'signature' network-level brain activity aberrations in these patients. This knowledge will be applied towards a novel treatment strategy based upon a physiologically-defined computational model of neurological circuit function integrated into a closed-loop system. A complementary approach is to develop novel state-of-the-art technology for safe, but high spatiotemporal resolution recording and stimulation to multiple brain regions simultaneously for clinical application. This device platform will far exceed the capabilities of any technology platform ever created and will be available for experimental studies in non-human primates to obtain critical knowledge on mechanisms and will simultaneously inform human clinical studies to validate new recording/stimulation strategies for potential amelioration of human neurological and neuropsychiatric disorders.

J. Defense Forensic Science Center Research and Development Program

The goal of this program, co-managed by the Life Sciences Division and DFSC, is to enhance the capability of forensic science applications in traditional law enforcement/criminal justice purviews and in expeditionary environments. In FY16, six active projects were co-managed by ARO and DFSC under this program. One project aims to optimize an RNA-based body fluid multiplex identification system by developing a differential DNA/RNA co-extraction isolation protocol for the separation and analysis of non-sperm and sperm fractions in sexual assault evidence (i.e., prior to DNA profiling and identification of body fluid of origin). The proposed system will enhance forensic capabilities of DFSC and civilian law enforcement by conclusively identifying all forensically relevant biological fluids in a given sample. The proposed system will also be seamlessly compatible with current DNA typing technology by enabling co-extraction of both DNA and RNA from the same

forensic sample. Another effort is evaluating ground-, air- and satellite-based sensing technologies for their performance in human grave detection using an experimental study site in east Tennessee, with the main data focus on LIDAR and spectral imaging. The development of remote methods to locate clandestine gravesites will increase gravesite detections per year, reduce recovery cost per individual, and enable the DoD to closely monitor additional gravesites in non-permissive environments, thereby maintaining the grave's chain of custody. Another effort is developing a Next Generation Sequencing-based autosomal short tandem repeat (STR) allelotyping capability. The proposed platform will enable STR analysis and mitochondrial DNA to be analyzed concurrently, along with other genetic markers that can provide information on the physical characteristics and ancestry of an individual, providing enhanced forensic information to examiners. The development of a set of algorithms and software tools to discover the make and model of a digital image's source device by forensically analyzing the image itself is the goal of another project. If successful, this effort would provide a new capability to Army and DoD forensic examiners, as there is currently no scientific method available to make this determination. Another effort is focused on increasing DoD's ability to identify human remains by creating new kinship and ancestry algorithms that increase the efficiency of identifying old and/or highly degraded remains. The intent of this project is to be able to identify remains of service members when only distantly related individuals are available, as is the case for many remains from WWII, Korea, and Vietnam. The final project is developing a spray-on, peel-off, nondestructive coating for trace chemical collection from surfaces and a detailed method for its use. This effort will provide DFSC with an enhanced capability to collect a wide range of trace chemicals from a variety of surfaces, including porous materials which are traditionally challenging to analyze.

K. DARPA Biological Robustness in Complex Settings (BRICS) Program

The goal of this DARPA program is to develop the fundamental understanding and component technologies needed to engineer biosystems that function reliably in changing environments. A long-term goal is to enable the safe transition of synthetic biological systems from well-defined laboratory environments into more complex settings where they can achieve greater biomedical, industrial and strategic potential. Within this program, the Life Sciences Division co-manages one project which seeks to develop new approaches to manipulate unculturable and undomesticated microbes through *in situ* genome engineering. These technologies have the potential to discover new genetically tractable microbes with novel manipulable capabilities for applications in agriculture, bioremediation, bioenergy, biodefense and health. This project further focuses on the development of a generalizable method to limit robustness of the genetic code using overlapping genetic recoding. The results from this genetic study will be useful as a defense against targeted efforts to inactivate a gene or pathway of interest or to remove the engineered safety mechanisms associated with a synthetic function.

L. DARPA Hand Proprioception and Touch Interfaces (HAPTIX) Program

The goal of this program is to create a prosthetic hand system that interfaces permanently with the peripheral nerves in humans. ARO Life Sciences co-manages HAPTIX projects focused on tapping into the motor and sensory signals of an amputee's residual arm, allowing them to control and sense an advanced prosthesis via the same neural signaling pathways used for intact hands and arms. Direct access to peripheral nerves would allow users to move and receive sensation like a natural hand such that it creates a sensory experience so rich and vibrant that users would want to wear their prostheses full time. By restoring sensory functions, HAPTIX also aims to reduce or eliminate phantom limb pain, which affects about 80 percent of amputees. The program plans to adapt one of the prosthetic limb systems developed recently under DARPA's Revolutionizing Prosthetics (RP) program to incorporate interfaces that provide intuitive control and sensory feedback to users. These interfaces build on advanced neural-interface technologies being developed through DARPA's Reliable Neural-Interface Technology (RE-NET) program.

M. DARPA Biological Control Program

The goal of this program is to build new capabilities for the control of biological systems across scales—from nanometers to centimeters, seconds to weeks, and biomolecules to populations of organisms—using embedded controllers made of biological parts to program system-level behavior. The program is co-managed by the Life Sciences Division, which involves participation and leadership in proposal evaluations, selections, monitoring,

and site visits. The program is focused on applying and advancing existing control theory to design and implement generalizable biological control strategies analogous to conventional control engineering (e.g., for mechanical and electrical systems). Specifically, the Biological Control program will demonstrate tools to rationally design and implement multiscale, closed-loop control of biological systems, through the development of biological controllers, testbeds to evaluate control of system-level behavior, and theory and models to predict and design effective control strategies. If successful, the resulting advances in fundamental understanding and capabilities will create new opportunities for engineering biology.

N. DARPA Restoring Active Memory (RAM) Replay Program

The goal of this program is to develop new closed-loop, non-invasive systems that leverage the role of neural "replay" in the formation and recall of memory to help individuals better remember specific episodic events and learned skills. ARO Life Sciences co-manages RAM Replay projects focused on non-invasively detecting, modeling, and facilitating real-time correlates of replay in humans, leveraging not only neurophysiology, but also other factors including physiological state and external elements in the surrounding environment. Research challenges include validating assessments and intervention strategies through performance on DoD-relevant tasks, rather than relying on conventional behavioral paradigms commonly used to assess memory in laboratory settings. Using the new knowledge and paradigms for assessing memory formation and recall, the program seeks to improve performance of complex skills by healthy humans.

O. Minerva Research Initiative (MRI) Topic: Studies of Non-State Adversarial Organization, Ideologies, and Strategies

The objective of this MRI topic is to examine the relationship between trans-national terrorist ideologies and intergroup conflicts. Areas of particular interest include: the interaction between political dynamics on the ground and the goals and ideologies of non-state adversarial groups; the role of new media technologies in recruitment, radicalization, and de-radicalization in insurgent movements; the spread of insurgent ideologies across culturally diverse populations; and the role of non-rational decision making (e.g., values, morals, trust, belief and emotions) in the collective behavior in insurgent groups and how best to represent non-rational decisions in computational models of collective and group behavior. This research, if successful, will provide better understand the dynamics of non-state adversarial organizations, their underlying motivations and ideologies, how they organize, how they recruit and retain members, and how they evolve and adapt in the face of new challenges. In addition to overall network characterization, there is an urgent need to be able to locate the points of influence and characterize the processes necessary to influence populations that harbor terrorist organizations in diverse cultures as well as individuals who identify with terrorist group figures of note. A better understanding of neuro-cognitive systems responsible for the processing of socio-cultural and other environmental cues is crucial both to research and to a whole range of practical situations. The BAA for this MRI topic was released in FY08, FY09, FY10, FY11, FY12, FY13, FY14, FY15. Project selection and funding began in FY09. There were eight active projects pursuing research under this topic in FY16.

P. Minerva Research Initiative (MRI) Topic: Science, Technology, Political, and Military Transformation in Asia, Eurasia, & Latin America

The objective of this MRI topic is to explore the social, cultural, and political characteristics and implications of trends and developments in growing military powers (e.g., China, Brazil, Russia), as well as in supporting technological and industrial sectors as they relate both to security policy and strategy and to the broader evolution of society. This research area utilizes a wealth of unclassified information, not generally known beyond a small circle of researchers, about military, technological and scientific development (including information that is published by governments in these states, but difficult for scholars outside of them to locate or access). Access to these data will facilitate research into trends in military and technology development and promise to provide valuable insights into the workings of an important and influential power. The coding of this data into a comprehensive relational database that will be made available to scholars beyond this project combined with the projects continued focus on building a community of researchers collectively engaged in understanding these aspects of modern international military development. The breadth and depth of topics

offers insights into the dynamics and intersections of industry, science, technology, political governance, and social structures that shape modern military organizations and indicate why some countries emerge as military powers, while others remain stagnant. The research will inform a wide range of decisions relevant to national security and economic policy, from diplomacy to science and technology planning to military resource allocation. The BAA for this MRI topic was released in FY11, FY12, FY13, FY14. Project selection and funding began in FY12. There were six active projects pursuing research under this topic in FY16.

Q. Minerva Research Initiative (MRI) Topic: Security Implications of Energy, Climate Change, and Environmental Stress

The objective of this MRI topic is to establish new theories and models of societal response to external pressures that shape sociopolitical outcomes. Of particular interest are stressors related to environmental stressors. Until recently, most studies of these phenomena have focused on historical case studies and domain-specific policy development (*e.g.,* establishing policy on carbon footprint reduction, cross-national cooperation to manage water resources, developing policies to improve food security). In the last few years, social scientists began to quantitatively explore the intersection among these factors by asking how changes in the environment alter risk perception and human behavior, and affect the availability and distribution of essential resources (*e.g.*, water, grains) and geomorphologic changes (*e.g.*, desertification). Affected societies experiencing these shifts must work to mitigate competition over increasingly scarce resources, which can otherwise contribute to the emergence of political and social unrest. In addition, worldwide increases in demand for nonrenewable energy and resource access have the potential to limit the ability of societies to sustain current economic and social standards of living. This MRI supports research that will contribute to fundamental understanding of the implications of these exogenous stressors from a global security perspective. This research will likely aid DoD decision-making in terms of the development of improved methods for identifying and anticipating potential hot zones of unrest, instability and conflict and help in strategic thinking about resource allocation for defense efforts and humanitarian aid. The BAA for this MRI topic was released in FY10, FY11, FY12, FY13, and FY14. Project funding and selection began in FY12. There were four active projects pursuing research under this topic in FY16.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Life Sciences Division.

A. Engineering Nanoscale Protein Containers
Professor Danielle Tullman-Ercek, Northwestern University, Single Investigator Award

Polyhedral protein-based microcompartments are ~125 nm enclosed scaffolds that natively encapsulate enzyme pathways in bacteria, and are promising structures for the bacterial production of chemicals and pharmaceuticals (see FIGURE 2). They hold great potential for future applications, including *in vitro* nano-containers and drug delivery devices, due to the precise structure and size of these protein assemblies. Segregating reactions in such compartments offers multiple potential advantages: (i) sequestration of toxic or highly reactive substrates or intermediates; (ii) enhanced kinetics for product synthesis; (iii) creation of unique interior environments; and (iv) avoidance of off-pathway competing reactions. Recently, encapsulation of a synthetic, two-enzyme ethanol production pathway in a microcompartment resulted in higher yields compared to an unencapsulated pathway *in vivo*. This result opens the door for additional pathways to be compartmentalized, but hurdles remain before this technique can be widely applied either within the cell or in other contexts. It is not known how to adjust the number, size, shape, and cargo loading of microcompartments, and the ability to tune these parameters will be essential for optimal performance. For example, yields are expected to correlate with the number of microcompartments per cell, yet there are no known mechanisms for altering the microcompartment concentration, and any imbalance in protein shell components leads to misformed structures or aggregation. Moreover, enzyme targeting to the interior of the microcompartment is only understood for single enzymes; competition between multiple enzymes and control over stoichiometry is as yet unexplored. Finally, the rules governing assembly and cargo encapsulation *in vitro* are unresolved.
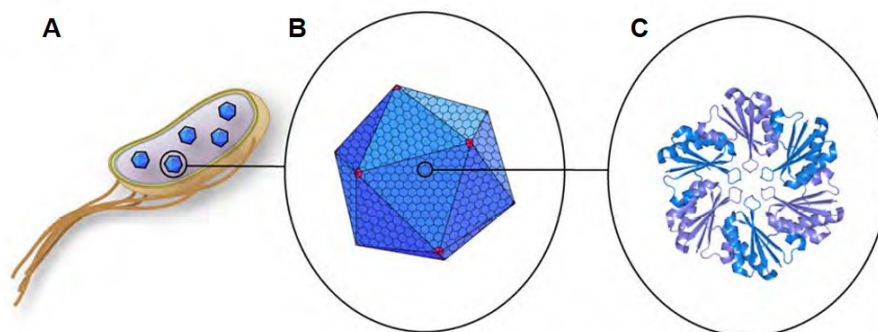

FIGURE 2

Bacterial microcompartments. (A) These bacterial structures compartmentalize enzyme reactions in cells. (B) The structures are polyhedral and consist of multiple constituent proteins that form vertices (red) and facets (blue). (C) The facets consist of hexamers of a single shell protein.

To advance the translation of these scaffolds to applications for synthetic biology and beyond, Prof. Danielle Tullman-Ercek at Northwestern University is developing a detailed fundamental understanding of microcompartment regulation and assembly, as well as exploring approaches to precisely control the amount and stoichiometry of enzymes loaded within these structures.

In FY16, control of the loading of protein cargo within the 1,2-propanediol utilization microcompartment of *Salmonella enterica* was demonstrated using two strategies: (i) by modulating the transcriptional activation of the microcompartment container and (ii) by coordinating the expression of the microcompartment container and the cargo proteins. These strategies allow general control over the loading of cargo proteins within microcompartments and represent an important step toward tuning the catalytic activity of bacterial

microcompartments for increased biosynthetic productivity. This scientific accomplishment was published in the Journal of Molecular Biology in July 2016.

Professor Tullman-Ercek will build upon these results to explore the range of shell protein expression levels that allow for proper mirocompartment assembly in cells and to identify requirements for microcompartment shell formation *in vitro*. Protein-based containers could advance technologies supporting several new Army and DoD capabilities, including production of specialty chemicals, drug delivery and nanomaterial fabrication. When used in bacteria, engineered microcompartments could facilitate biological production of previously incompatible chemicals. Beyond the cellular environment, this research could lead to creation of "organelles" within artificial cells, offering spatial sequestration of components as needed for the design of these systems. Artificial cells hold promise for further expanding the set of conditions at which biological syntheses can be performed to produce specialty chemicals or materials. The research will also inform the controlled assembly of protein-based nanoscale structures. Such assemblies could be used as nanoscale bioreactors, which could carry out enzymatic reactions in non-aqueous solvents to enable production of polymers, explosives, and other chemicals that normally require tremendous infrastructure to produce synthetically.

B. Imaging Efflux Machineries for Metal Defense in Live Bacteria
   Professor Peng Chen, Cornell University, Single Investigator Award

Microorganisms must withstand and adapt to a variety of environmental stressors in order to maintain their viability. One common environmental stress is the presence of metals in the environment. While metals such as copper and zinc are required for a number of essential functions and enzymatic reactions in the cell, an excessive concentration of these metals can be toxic to the cell promoting the formation of oxygen free radicals leading to excessive DNA damage and ultimately cell death. To counter this, there exist a family of tripartite pumps in *E. coli* that are specific for actively transporting and conferring resistance to a number of metals and organic toxins. The gene products of the CusCBA operon has been shown to mediate resistance to copper and silver forming a multi-subunit complex traversing the periplasmic space between the inner and outer membranes forming a channel that actively pumps these metal cations from the cytoplasm to the extracellular space. What remains poorly defined is how the subunits of this efflux are dynamically assembled.

On the basis of preliminary studies, the goal of this research is to test the hypothesis that CusCBA exists in a dynamic disassembly-assembly equilibrium and in response to increasing cellular Cu levels, shifts toward the assembled $CusC_3B_6A_3$ form for more effective efflux. To test this, they are using the approach of nanometer-scale single-molecule tracking via time-lapse stroboscopic imaging in which the proteins will be tagged with a photoconvertible fluorescent protein in living cells (see FIGURE 3). This dynamic tracking will enable quantification of diffusion behaviors associated with different assembly forms of the complex. Chen has demonstrated that the diffusive behavior of a fluorescently tagged form of the CusA protein can be decomposed into two major components: one faster (free, dissociated CusA protein) and one slower (CusA protein assembled into the CusCBA complex). Upon stressing the cells with copper, a population shift from the fast-diffusing component to the slow-diffusing component is observed within 30 minutes supporting the hypothesis that copper can induce a dynamic shift in the assembly-disassembly equilibrium. Further, a kinetic analysis from the dynamic imaging data shows that the shift in the assembly forms result from a combination of an increase in the assembly kinetics and a decrease in the disassembly kinetics. Tracking experiments using CusB variants that remove the copper-binding cysteines show that the observed assembly shift under copper stress is abolished indicating that copper binding to the CusB protein is required for the dynamic assembly shift. Collectively, these experiments provide a clearer understanding of how bacteria efficiently respond to the presence of metallic toxins through the mobilization of specific protein complexes.
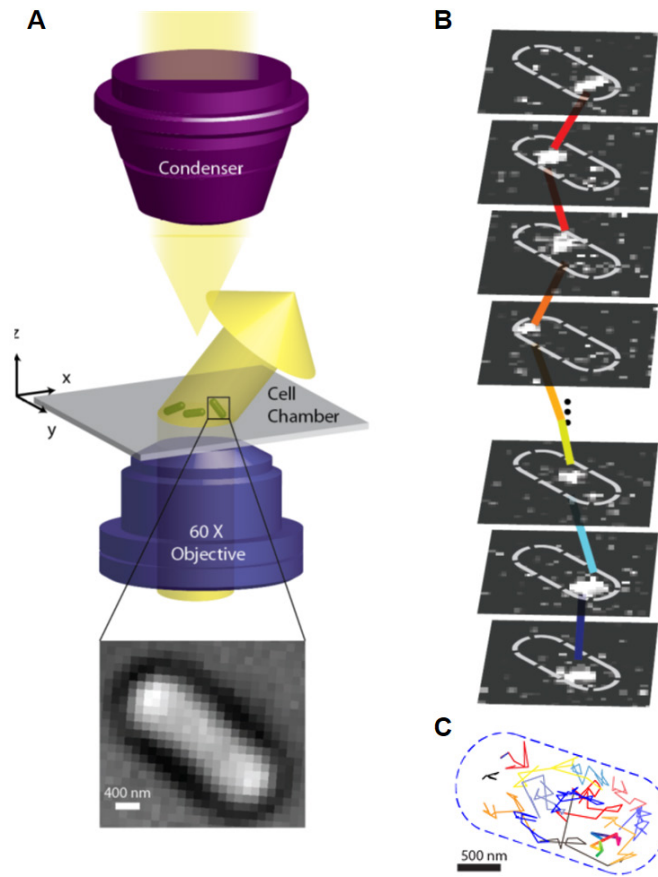
FIGURE 3

Time-lapse stroboscopic imaging of intracellular proteins. (A) Schematic setup of the fluorescence microscopy, on which a transmission image of an *E. coli* (bottom) cell can be first taken. Then single-molecule tracking via stroboscopic imaging can be performed. (B) A series of stroboscopic fluorescence images of a single protein molecule, tagged with photoconvertible fluorescent protein. The bright spot in each image is a single protein, which moves in time (from top to bottom). In each panel, the center position of the protein molecule can be localized to down to a few nanometer accuracy. (C) Many motion trajectories (colored lines) of individual CusA molecules are overlaid on top of the cell boundary (dashed line).

C. Computational Models of Cultural Meaning and Social Interaction
Professor Dawn Robinson, University of Georgia, Single Investigator Award

The objective of this research is to develop new dynamic models linking identity, culture, affect, and action leveraging a large cross-cultural database. Cultural competence is critical to effective decision-making in the dynamic and diverse environments in which military operations are carried out. Failure to recognize cross-cultural differences can lead to communication failures and the unintended escalation of conflict, but achieving cultural mastery has traditionally required intensive and extended immersion in the language and practices of the group, which is not always plausible when events are rapidly developing and involve multiple diverse groups.

In FY16, Professor Robinson's laboratory generated a compelling new approach through Affect Control Theory (ACT) to mathematically model meanings assigned to identities and actions in different cultures, enabling the ability to simulate and predict how interaction will unfold. In this approach the actors and behaviors are mathematically modeled in three dimensions of meaning (power, morality, and activity), which Robinson has demonstrated can be rapidly estimated for thousands of actors and behaviors in any cultural group using crowdsourcing approaches. Robinson has also developed equations to represent cultural rules for interaction, which predict the likelihood of combinations of actors and actions based on the degree to which the three dimensions of meaning for the actor and actions correspond. When correspondence is low, actors experience negative affect, referred to as deflection. Deflection signals that behavior is viewed as inappropriate for an actor

and disrupts the interaction. To lower deflection, others will change their behavior toward the actor in order to restore disrupted interaction. These changes occur with little conscious effort and make sense among members of the same culture who share meaning and the same rules for interactions. Because meanings and interaction rules are culturally dependent, however, when actors come from different cultures the lack awareness of the different rules and meanings governing each party's behavior can create unintended disruptions. In these situations, the changes actors take toward one another in attempts to restore interaction can fail, and interaction becomes increasingly unpredictable and volatile as parties are unable to resolve deflection. To test the viability of the approach, the research team developed equations for Egyptian and U.S interaction to simulate 13 million interaction episodes. The results indicate considerable overlap in the cultural meaning of actors and behaviors across the cultures, but sensitivities in the equations suggest that certain combinations of actors and behaviors are likely to increase deflection when they are enacted in cross-cultural settings (see FIGURE 4).
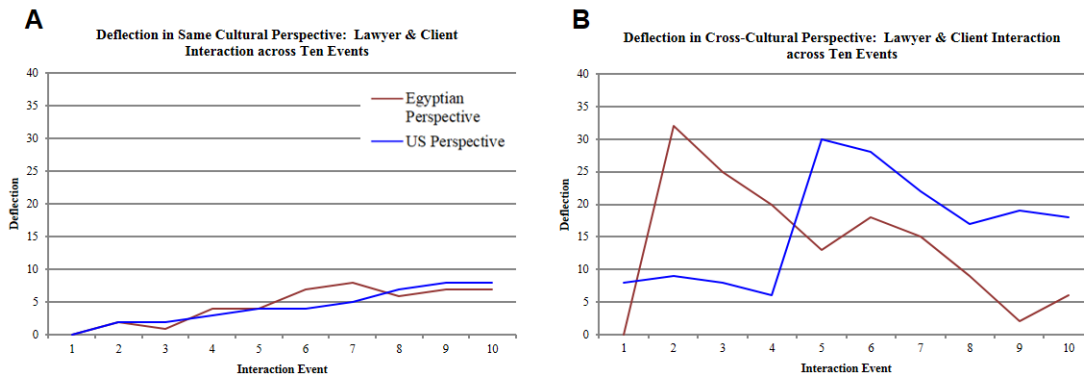
FIGURE 4

Affect Control Theory. The lines indicate level of deflection with a theoretical range of 0-40 for (**A**) same culture interaction and (**B**) cross-cultural interaction. As the graph shows, deflection across the same types of interaction (lawyer-client) generate significantly greater deflection when individuals from different cultures are interacting, even though the roles are the same and the meanings of those roles are very similar across the cultures. In this result, the mathematical equations representing interaction rules in each culture amplify the relatively small differences in meaning, creating the potential for conflict.

Because of these sensitivities, the equations that represent cultural rules for interaction, can amplify even small meaning differences in cross-cultural interactions, creating highly volatile interaction episodes. In some instances, the simulations indicated that the volatility cannot be managed by the actors through reparative attempts to lower deflection and restore the interaction. In these instances, conflict can rapidly spiral out of control, exacerbating distrust and even provoking violence. This research breaks new ground in scientific understanding of the relationships between cognition, affect, and culture that shape social interaction. It is also enabling the development of new tools to rapidly predict how actors from different cultures will behave toward one another, as well as how they will interpret the behavior of others, without requiring cultural mastery. This research has potential to sharply reduce cross-cultural conflict and improve the effectiveness of decisions in situations involving diverse groups.

D. Neurodynamics of Social Status
Professor William Kalkhoff, Kent State University, Single Investigator Award

While substantial scientific advances have been made in biometric measurements, including brain imaging and researchers have made great strides in understanding these states in isolated individual humans, little is understood about the relationship between social dynamics and biophysiological states. Professor William Kalkhoff has generated new discoveries that are advancing scientific understanding of both social dynamics and how these dynamics relate to brain patterns. Drawing on research on human problem-solving and brain activity, the research team's new theory identifies critical areas of brain activity in problem-solving groups, which corresponds to social dynamics. Remarkably, the research shows that when individuals work in groups, as opposed to in isolation, activity levels in these critical regions vary, depending on their status in the group. Kalkhoff and his colleagues identified the left dorsolateral prefrontal cortex (DLPFC) as a critical region. In a series of innovative experiments using EEG technologies to operationalize and track brain activity, the

researchers manipulated the status of a group member and tracked brain activity over several regions believed to be related to problem-solving. The results indicate that in the left DLPFC, group members who believe they are higher status than other group members, exhibited significantly more brain activity. This is particularly insightful, because the status of the members was manipulated, as opposed to actual – when members believed their status was lower, brain activity in this region was significantly lower. Moreover, status was explicitly de-coupled from the problem-solving task, such that members believed there was no reason to think that a higher status person (based on rank) had greater ability to solve the problem.
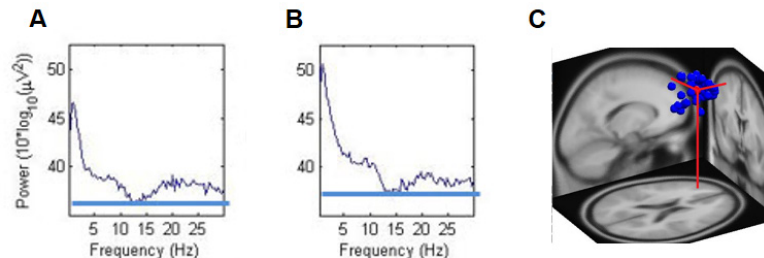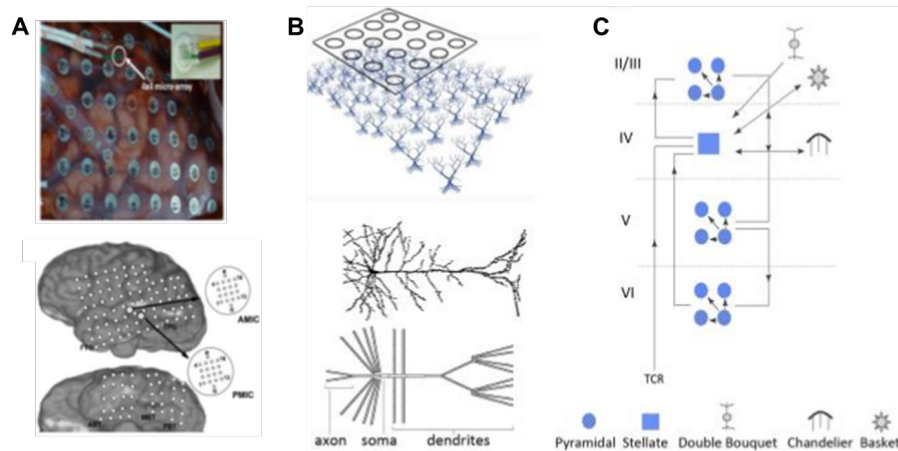

FIGURE 5

Isolating neurodynamics of brain activity as a function of status in problem-solving groups. The results revealed a distinct difference in Alpha Power in the Dorsolateral Prefrontal Cortex (DLPFC) that vary with group member status. The panels illustrate (**A**) lower power among higher status actors detected at around the 12Hz frequency level compared to (**B**) lower status actors, as represented by the blue horizontal line. Lower Alpha Power corresponds to greater brain activity in this region, indicating higher status actors take on a heavier burden cognition. (**C**) This project was also able to isolate components of the DLPFC associated with activity. In this panel, blue spheres represent the individual components, with the red intersection showing the grand mean for all participants.

This research represents the first time that social attributes, such as status, and social interaction (in this case, a group problem-solving scenario) have been linked to neurodynamics. It also reaffirms research based on less precise instrumentation that higher status group members (such as group leaders) engage in more cognitive work as a group seeks to solve problems. In ongoing research, Kalkhoff is conducting further experiments to assess the temporal development of these patterns. The scientific discoveries that Kalkhoff is generating promise new ways to detect the emergence of influential group members members and how members of a group synchronize their cognitive work in an effort to accomplish their goals. It is also opening new avenues for understanding the relationships between biophysiological states and social dynamics.

E. Multi-scale Dynamics of Cortical Adaptation for Human Auditory Detection
Professor Dana Boatman, Johns Hopkins University, Single Investigator Award

The ability to detect and respond rapidly to novel sounds is critical for survival. Animal electrophysiology studies have shown that short-term cortical adaptation facilitates detection of novel sounds even when not actively attending to the environment. Adaptation refers to reduced neural activity for repeated or ongoing (background) sounds and is a form of experience-dependent cortical plasticity. However, the temporal properties of adaptation in human cortex are poorly understood. The dearth of high resolution human neural data, coupled with morphological differences between human and animal auditory cortex, has hampered efforts to develop realistic computational models of cortical auditory processing. Computational neural network models of sensory processing have focused mainly on visual cortex and have been largely unexplored in auditory cortex. Moreover, development of neural network models is rarely based on in vivo data, leading to potentially unrealistic representations of sensory processing. In FY15, Professor Boatman and colleagues developed a multi-compartmental model to simulate short-term adaptation of local cortical activity, including firing patterns, and used to analyze data from human electrocorticography recordings during active listening in awake human subjects (see FIGURE 6).

FIGURE 6

Human electrocorticography and neocortical modeling. (**A**) Intra-operative photo of macro- and micro-electrocorticography grid array placement. Bottom, left hemisphere lateral and mesial 3D MRI reconstruction showing implanted arrays and coverage of superior temporal gyrus. (**B**) Schematic of Layer II/III neuronal network in modeled minicolumn with modeled micro-elements above to represent 4x4 micro-electrode recording array on cortical surface. Note: inter-cell and inter-electrode distances are rescaled for visualization; actual scale factor ratio is approximately 50:1. Bottom, in vivo pyramidal cell (top) and modeled pyramidal cell (bottom). (**C**) Diagram of cellular architecture and connectivity in modeled minicolumn. Omitted for visibility are: Layer IV pyramidal cells, Layer I containing pyramidal apical dendrites from Layers II/III; inhibitory connections to other layers, and thalamic reticular nucleus input.

In FY16, additional analysis tools were utilized to determine the extent that cross-frequency coupling between brain regions plays an important role in coordinating neuronal computations underlying human perception, learning and memory. Four separate methods for measuring phase/amplitude coupling of theta (4-7 Hz) and high-gamma (70-150 Hz) in intracranial electrocorticographic (ECoG) recordings were directly compared, which is the first time that all four methods have been applied to the same human ECoG datasets. Results suggest that all four methods yielded significant increases in phase/amplitude coupling during a passive listening task. However, the pattern of coupling differed across methods suggesting that the choice of which phase/amplitude coupling method to use should be guided by the research questions and experimental conditions and that a combination of PAC methods may be the best approach. Professor Boatman's research is enabling realistic biophysical models of neural network dynamics associated with real-world listening conditions that include degraded, competing and multimodal (auditory-visual) inputs, as well as fluctuations in listener state (attention, fatigue). These advances are being achieved through the development of new analytical tools that will be available to the field of human auditory neurophysiology and will help to uncover mechanisms and temporal dynamics of adaptation in human cortex.

F. Fracture and Deformation in Trabecular Bone: Anisotropy, Hierarchy, and Scaffolds
   Professor Julia Greer, Caltech, AICB (UARC)

Trabecular bone has proven very difficult to study and model experimentally because of its heterogeneity, anisotropy, and multi-scale mechanics. The objective of this research is to elucidate the relative importance of various contributing factors in bone fracture, (i.e., underlying microstructure and hierarchical organization of the constituents (fibrils, collagen fibers, amorphous and mineral phases), anisotropy) and the drivers for the trabecular bone strength and damage resistance.

In human bone, an amorphous mineral serves as a precursor to the formation of a highly substituted nanocrystalline apatite. In their recent work, Professor Greer and colleagues showed by using transmission electron microscopy that 100–300 nm amorphous calcium phosphate regions are present in the disordered phase of trabecular bone. Nanomechanical experiments on cylindrical samples, with diameters between 250 nm and 3,000 nm, of the bone's ordered and disordered phases revealed a transition from plastic deformation to brittle failure and with a strength at least a factor of two higher versus the smaller samples (see FIGURE 7). The team postulate that this transition in failure mechanism is caused by the suppression of extrafibrillar shearing in the

smaller samples, and that the emergent smaller-is-stronger size effect is related to the sample-size scaling of the distribution of flaws. The result of this effort will help guide the design and creation of better protective systems, minimizing the impact to bone, and develop more mechanically resilient artificial bone.
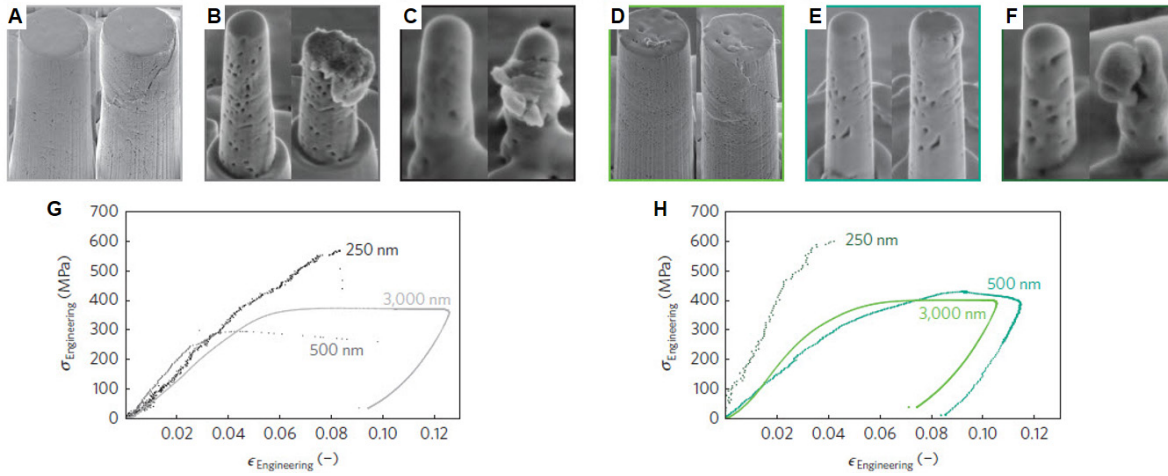

FIGURE 7

Uniaxial compression results of ordered and disordered pillars. Pre- and post-compression (left and right, respectively) images of ordered (**A–C**) and disordered (**D–F**) pillars showing samples exhibiting distinct failure modes: shearing in A,B,D and brittle failure in C,E,F. Characteristic stress versus strain responses of the ordered (**G**) and disordered (**H**) 3,000, 500 and 250 nm pillars.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Spore DNA Extraction Techniques Utilized in Microbiome Studies
Investigator: Professor Peter Setlow, University of Connecticut, Single Investigator Award
Recipient: Shoreline Biome, Inc.

Bacteria of Bacillus and Clostridia species can grow vegetatively in an environment containing an abundance of nutrients. However, when nutrients are scarce, these species can undergo a process called sporulation where cells become surrounded by a number of protective layers resulting in a spore with practically unnoticeable level of cellular metabolic activity and extreme resistance to many environmental insults including heat, desiccation and chemical treatment. This highly resistant spore, then, presents a significant challenge if one wishes to identify and analyze its internal biochemical components. ARO-funded research performed over a number of years by Professor Setlow has been focused on the challenge of understanding the metabolic programming of Bacillus species in their sporulated state and the cellular and metabolic adaptations that Bacillus undergoes as the cell transitions into and out of the spore state. Through this research, a methodology was developed by which mechanical breakage of spores has provided a means of freeing the contents of the spores for analysis.

This facet of Professor Setlow's research is now contributing to the comprehensive genomic analysis of the human gut microbiome, which detects and quantifies the hundreds of different types of bacterial DNA found in a typical microbiome sample. Bacterial spores are present in the gut microbiome, but are frequently under-represented or not detected in DNA assays because their protective layers prevent release and detection of their DNA. The problem is difficult to solve because harsh treatments like boiling can open the spores, but at the same time they also destroy the DNA. A Connecticut start-up company nearby Professor Setlow's laboratory, Shoreline Biome, has leveraged his research in spore breaking for their genomic studies aimed toward cataloging the contents of the human gut microbiome. Shoreline Biome researchers have successfully obtained high quality genomic DNA from spores using this unique mechanical breakage method. In consultation with Professor Setlow, Shoreline Biome is developing a prototype high-throughput instrument that greatly improves microbiome analysis by breaking open all microbes, including spores, releasing the DNA for downstream high-throughput genomic analysis. Shoreline Biome is located at the Technology Incubation Program on the University of Connecticut campus in Farmington, CT, where they manufacture molecular biology kits, software, and instruments for the analysis of the microbiome. The spore breaking technology provides an unprecedented, comprehensive view of the microbes that inhabit humans, enabling groundbreaking research with vast potential for understanding health and disease that is expected to lead to new medical advances.

B. Artificial Skin Models for Studies of the Human Skin Microbiome
Investigator: Professor David Karig, Johns Hopkins University/Applied Physics Laboratory, MURI Award
Recipient: NSRDEC

Results from MURI-funded researcher at Johns Hopkins University/Applied Physics Laboratory (JHU/APL) have transitioned to NSRDEC for follow-on research to utilize artificial skin models for studies of the skin microbiome. Recent experiments by JHU/APL using these skin equivalent models have identified how common skin bacteria use different resources to enable their growth and interspecies interactions. This understanding will facilitate recognition of unhealthy bacteria and allow their manipulation to enable new tools for disease prevention. JHU/APL results are being incorporated into NSRDEC models for further skin microbiome studies aimed primarily toward testing of antimicrobials that are tethered to textiles. One of the limitations of the *in vitro* skin models is the limited shelf life of the system due primarily to difficulties in attaining a reliable means of bacterial adherence to the artificial skin and acclimation of the bacteria when transferring the cells from liquid culture media to the skin model. In bringing this *in vitro* system into their laboratory, NSRDEC is currently in the process of developing a protocol and culturing conditions for a multi-species community that enables

improved bacterial adherence. The development of this protocol will be of great value to both JHU/APL and NSRDEC during the next phases of their respective research. In addition, this partnering enabled the successful development and installation of the first mammalian cell culture facility within the NSRDEC Warfighter Directorate. In total, this transition from JHU/APL to NSRDEC is leading to a more complete understanding of the dynamics of the skin microbiome and has the potential to enable new capabilities for rapid, on-site disease screening in garrison, of deployed soldiers and of partner nation personnel and citizens.

C. Moral Schemas, Cultural Conflict, and Socio-Political Action
   Investigator: Professor Steven Hitlin, University of Iowa and Professor Rengin Firat, Georgia State University, Minerva Research Initiative
   Recipient: CENTCOM,

Social science research is transitioned primarily as a knowledge innovation that transferred to policymakers, military decision-makers, and organizational leaders in the public and private sectors. Often this occurs through briefings and workshops, with specific objectives and results in the form of policy and operational decisions developed based on the knowledge that the recipient has requested and resourced. This focuses on developing new insights on how social values translate into political actions across diverse populations. The research team has proposed that when an individual's moral values are challenged, a chain between emotion and action is catalyzed. Challenges to moral values can arise when actors experience an external threat to the group to which they belong. The research team hypothesizes that challenges to moral values can arise from social threats (i.e., threats of repression) or physical threats (e.g., occupying the group's territory). Moreover, when the challenges occur, they hypothesize that specific brain regions are activated that control emotion (ventromedial prefrontal cortex and amygdala). This activation, in turn, leads to heightened activity in the dorsolateral prefrontal cortex, an area of the brain responsible for rational processes, as actors try to address this moral conundrum. The result of this cognitive processing is decisions regarding whether and how to act. In Phase I of this research, the Professor Firat collected data on moral values, threat scenarios, and perceptions of the threat sources at a global level to establish a basis for Phase II experiments on brain responses and ensuing behavioral decisions.

Professor Firat's analysis of the Phase I data revealed that the majority of citizens in the Middle East and North Africa hold negative views of ISIL and also that religious extremism is not a factor in public support for ISIL or a reason given for joining ISIL. In a data drill-down, the analytic results also indicate that both Iraqis and Syrians overwhelmingly view ISIL negatively, but also overwhelmingly view foreign military intervention unfavorably, despite inability to drive back ISIL forces independently. Both ISIL and foreign military intervention are potential threats that challenge moral values, generating challenges for developing effective operational strategies. Professor Firat's analysis, based on systematic social scientific research, is the first to reveal the sensitivity to foreign intervention when a nation faces and is unable to independently overcome aggressive threats arising from internal insurgency, revealing the complexity of developing effective strategies.

Professor Firat's research was briefed with CENTCOM through a Strategic Multilayer Assessment reach back cell to respond to requests by CENTCOM to better anticipate opinions developing in the Middle East as ISIL forces are facing defeat. The research has been operationalized by CENTCOM in simulations to explore the future of Syria to predict how different external and non-state actors might seek to achieve their goals and deny those of other in shaping Syria's future trajectory. The reach back effort and simulations are being used for CENTCOM strategic development in this volatile region of the world.

D. A Computational Model of Resources and Resiliency
   Investigator: Professor William Rivera, Duke University, Minerva Research Initiative
   Recipient: USASOC

This research is developing new computational models and simulators to rapidly assess drivers that affect the mediation of conflict in a region, including environment, economics, technology, and political factions. The research also examines gaps in proposed operational strategies that may impede recovery in politically volatile regions. Professor Rivera is developing the models through comprehensive surveys of existing research and integration of databases on state fragility and conflict events in the Middle East. These data are complemented with primary data on (i) elements of national power, using the Diplomatic, Informational, Military, Economic

framework, (ii) regime propensities for risk aversion, and (iii) resource availability using thePower, Military Economic, Social, Infrastructure, Information – Physical Environment, Time framework.

Professor Rivera's team has integrated this first-of-its-kind database into a comprehensive model and developed a dynamic Course of Action (COA) Simulator to generate scenarios and predict the likelihood of sociopolitical instability and insurgency in the Middle East across these scenarios. The results have revealed path-breaking insights on the relative risk of insurgency for different states in the region, as well as their capacities to respond to emerging civil unrest and to insurgencies as their DIME and PMESII-PT profiles change. Additionally, the simulator enables rapid assessment of situations and identifies critical points of intervention in DIME and PMESII-PT assets that can inform development of effective strategy to achieve operational objectives.

Professor Rivera's laboratory has presented this research and the COA Simulator to USASOC, which then requested that Rivera develop and deliver a workshop, supported by USASOC, on Post-ISIL scenarios for USASOC units scheduled to deploy to regions of the Middle East in the near future. The workshop components entailed running advance scenarios in the region through the COA Simulator, followed by assembling panels of scientific experts to elaborate on the outcomes of the scenarios, COAs, and risks of the different strategies. Panel participants prepared white papers delivered to USASOC to support their upcoming mission. USASOC also received full access to the COA Simulator.

E. Protein Engineering Enables Alaskan Airlines Flight with Gevo-produced Wood-based Biofuel
Investigator: Professor Frances Arnold, Caltech, ICB (UARC)
Recipients: Gevo, Inc. and Alaskan Airlines

Pioneering protein engineering work conducted at the ICB over the past decade has led to the discovery of new enzymatic catalysts that has enabled the commercial production of a renewable replacement for the standard military fuel, JP-8. The pioneering approach used by the new-start company Gevo, developed novel enzymes that catalyze the biochemical conversion of plant sugars to isobutanol for conversion to JP-8 fuel. Gevo produces the only JP-8 fuel where the fuel is derived from renewable isobutanol. The Gevo-produced biofuels have been tested by Army TARDEC, demonstrated on Army Black Hawk helicopters and approved by the aviation standards body for use in commercial aviation. The research has now transitioned to Alaskan Airlines where the Gevo wood-based biofuel was first used on a November 2016 Alaskan Airlines flight.

F. Nanofluidic Analysis of Protein Transport, Adsorption and Kinetics
Investigator: Professor Sumita Pennathur, University of California - Santa Barbara, PECASE Award
Recipient: Alveo Technologies, Inc.

Nanofluidic systems offer unique capabilities for the separation and analysis of biological molecules. The advantages of nanofluidic technology are the result of underlying basic nanoscale phenomena, including entropy, sterics, electrostatics, electrodynamics, and adsorption dynamics, and in many cases, phenomena coupling two or more of these phenomena. For example, the unique coupled physics of the electric double layer, the resulting nonuniform velocity profile, hydrodynamic drag on an analyte, Brownian motion, steric interactions, and adsorption allows for unprecedented free-solution biomolecular separations based on size, mobility, and valence. Professor Pennathur is developing novel nanofluidic technology for the analysis of biological molecules. Specifically, as the recipient of a prestigious PECASE award, Professor Pennathur aimed to use nanofluidics to theoretically and experimentally investigate the effects of confinement, fluid velocity, surface conditions, labeling and nonspecific adsorption on protein transport, adsorption and kinetics.

During the course of the research effort, Professor Pennathur and her group discovered that non-specific protein adsorption to the nanochannel walls was a significant challenge preventing the type of analysis that had been proposed. To overcome these challenges, the team decided to take a step back from proteins to a much simpler system – ions – to carefully characterize their system for the analysis of charged species. In doing so, they discovered an approach to detect ions with extreme precision based on changes in conductivity. This then led the team to test whether a change in conductivity could be used to detect biomolecules such as DNA or proteins. They found that DNA could be detected with a very high degree of accuracy (as low as 100 copies in whole blood) by detecting the ions that are generated upon amplification of the DNA. For comparison, the sensitivity of current DNA detection platforms in whole blood for clinical diagnostic screening is 160,000 copies. These

results transitioned to Alveo Technologies for the development of sensors for the detection of various DNA sequences related to infection and disease. An initial target for the technology is rapid screening of donated blood in blood banks to ensure safety. The technology could be used to detect any DNA sequence of interest, and thus any target that contains DNA, including biological threat agents or engineered microorganisms.

G. Improving Outcome in Ischemia and Ischemia Reperfusion Injury
Investigators: Professor Mark Roth, Fred Hutchinson Cancer Research Center, Single Investigator Award
Recipients: Faraday Pharmaceuticals

The objective of this work is to prevent and mitigate oxidative damage caused by ischemia and reperfusion after tourniquet use, stroke, heart attack, organic transplant or trauma. Professor Roth has identified compounds that transiently and reversibly reduce oxygen consumption and metabolism in a variety of multicellular organisms, including humans, through reversible inhibition of the enzyme cytochrome c oxidase (see FIGURE 8). His group has demonstrated a 75% reduction in heart damage in a mouse model of chronic heart failure, and a 50% reduction in heart damage after induced heart attack in rats and pigs. Phase I human safety trials have been completed and no adverse effects were detected. In FY16, the FDA approved Phase II clinical trials to begin in the following year, and $20M in venture capital funding were obtained to begin these trials.
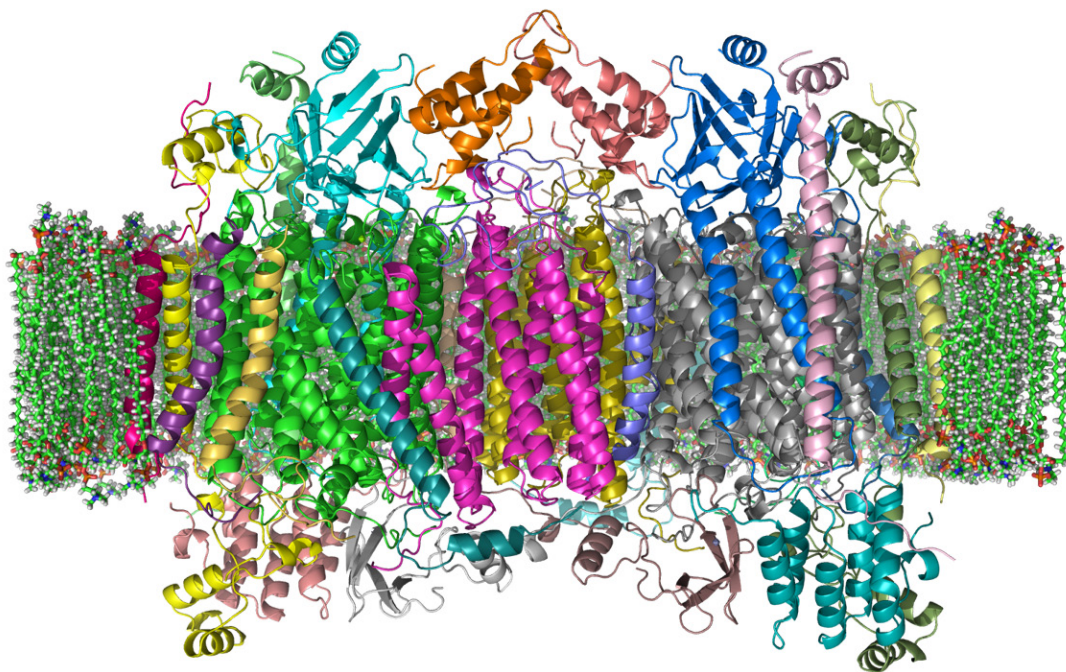

FIGURE 8

Cytochrome c oxidase. Professor Roth's laboratory has shown that blocking cytochrome c oxidase causes sudden, complete, and reversible metabolic shutdown in smaller eukaryotes.

H. Bio-Inspired Time Synchronization Transitions
Investigators: Professors F. Doyle, J. Hespanha, U. Madhow, and Y. Wang, UCSB, ICB (UARC)
Recipients: BioMimetic Systems, ARDEC, NSRDEC, ARL-SEDD

A collaborative Army-funded ICB research team, led by Biomimetic Systems, Inc., with UCSB as the academic partner, and with ARDEC and ARL-SEDD as the Army partners, has demonstrated an integrated set of technologies for mobile hostile fire detection at Fort Devens. The technology was demonstrated with live fire in situationally relevant scenarios in FY16, including multiple shooters and automatic weapon fire, to detect and localize shooters in essentially real time. The technologies demonstrated include individual biomimetic sensors for acoustic detection of gunfire, a specialized biologically inspired synchronization algorithm, and multi-sensor fusion algorithms for more reliable and accurate target detection/localization. Capabilities demonstrated include detection/localization of a single shooter by the sensor network with fully integrated display through the Nett

Warrior interface. The multi-sensor fusion algorithms provide for more reliable, actionable information via an improvement in accuracy, a reduction in false alarms, and a decrease in solution variability over individual acoustic sensors. The collaborative Army-industry-academic research team has transitioned this work to both the NSRDEC Nett Warrior team and ARDEC to transition and integrate these new technologies into the Nett Warrior platform so that situational information is distributed rapidly to both the soldier and command.

V.   ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Long-term Evolution of *E. coli*: Mutation and Vertical Transmission
Professor Steven Finkel, University of Southern California, Single Investigator Award

Microorganisms have an extraordinary capability to adapt and survive under harsh environmental conditions. Included among these stressors are conditions of starvation; over time, as energetically-rich nutrients become scarce, surviving bacteria in a culture acquire adaptive beneficial mutations that enable them to thrive on the resulting catabolic waste products of the culture and enter a phase of long-term survival. The steps leading to this phase in a laboratory experiment are the well-characterized lag and log phases where cells adapt to the presence of fresh nutrients followed by maximum growth rate (see FIGURE 8). Within 12 hours, all of the readily metabolizable media nutrients have been exhausted leading to a stationary phase. Over time, as expected, most (>90%) of the culture will then die; those that survive under Long Term Stationary Phase (LTSP) are those cells that acquired adaptive mutations; the kinetics of survival over extended time suggest that new genotypes appear over time as "waves" of GASP (Growth Advantage in Stationary Phase) mutations.
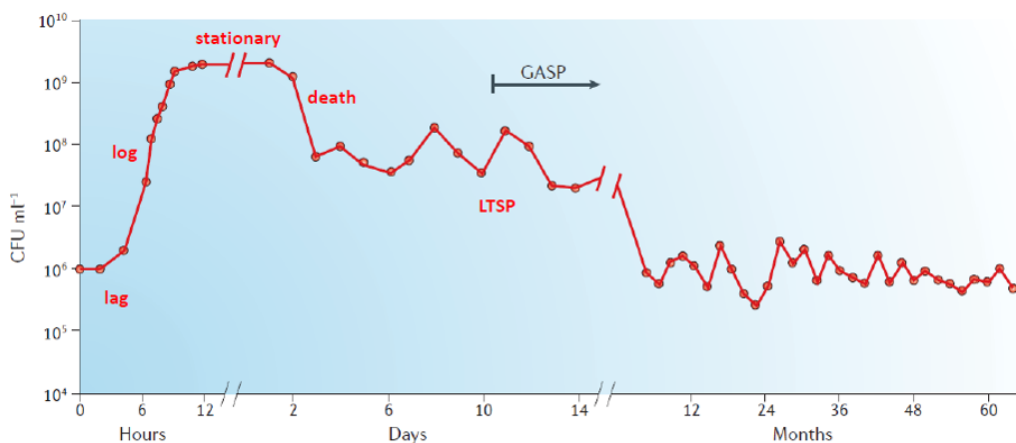

FIGURE 8

Five phases of bacterial growth during long-term survival. Bacteria can survive for long periods of time in batch culture, experiencing (1) lag phase, (2) log phase, (3) stationary phase, (4) death phase and (5) long-term stationary phase (LTSP). During LTSP, new genotypes appear over time, expressing new phenotypes, until they are replaced by newly evolved mutants.

While it is known that mutations do accumulate in GASP phase, little is known about the actual gene targets that are selected for mutation under these conditions. To address this, the Finkel laboratory has generated four parallel cultures of *E. coli* for 3.6 years without the addition of nutrients to examine the mutational signatures generated over time. An exhaustive genomic analysis of one of these culture lines up to 600 days show that a few specific mutational lineages dominate among the clones examined and that interestingly, new mutations accumulate in lineages over time, allowing them to apparently go extinct, only to re-appear later. The Finkel lab is currently examining the specific genes that are mutated within these signatures to assess the effects of specific mutations on fitness. Interestingly, there is a large number of mutations among the clones directed to the *hfq* gene, which encodes an RNA chaperone protein known to affect gene regulation. The team observed *hfq* mutations not only in the exhaustively analyzed culture line, but also among all four independent cultures: 25 different *hfq* mutations were observed, but just one specific allele dominates after days 10 and 20. Since *hfq* is a common target for mutation under LTSP, the Finkel lab will be directing efforts in FY17 toward understanding the apparent essential role of the Hfq gene product in early adaptive evolution. In addition, Finkel's group

noticed that there were over twice as many transposable insertion sequences (IS2 elements) present within clones taken from days 420 to 600 compared to the amount seen in the parental (day zero) culture. In FY17, the Finkel group will fully map the points of insertion of these elements and identify any genes that may have been disrupted by novel insertion.

Relative to well-mixed cultures in enriched broth that are typically constructed for many laboratory experiments in microbiology, the nutrient environment in LTSP more accurately reflects the types of conditions encountered in the natural world. In addition, the engineering of microbial systems of interest to the Army for future applications geared toward biosynthetic and material synthesis under fielded conditions will likewise be maintained under non-ideal and sparse growth conditions. A study of this type then will have great value for better understanding how microbes adapt to the austere condition of low nutrient availability and to develop rational strategies for maintaining their viability under these conditions.

B. Vocal Accommodation within Nonverbal Frequencies and Status Dynamics
Professor Joseph Dippong, University of North Carolina - Charlotte, YIP Award

The goal of this research is to develop a novel approach to understanding the biophysiological processes that may signal status dynamics in social groups. Recent research has demonstrated status represents a fundamental mechanism that organizes groups as members come together to work on tasks, advance shared goals, and solve collective problems. In fact, status hierarchies emerge in a matter of seconds in most groups, even when members are unfamiliar with one another and the particular characteristics they bring to the group. Those hierarches then structure who contributes and in what ways to the work of the group. When individuals are asked about how and why they adjusted their behavior, they are unable to explain it, suggesting that status organizing dynamics are largely non-conscious processes.

In this research, Professor Dippong is examining shifts in dominance over low frequency ranges of voice patterns in social groups (see FIGURE 9). Prior research provided evidence that speech at or above 500Hz is where normal speech that can be detected occurs and can be manipulated, while the range below 500Hz is not consciously managed and is difficult to interpret. Additionally, researchers have proposed that this lower frequency range carries social information (e.g., status, background, preferences) and is processed by the right brain, whereas verbal signals at the higher frequency range are processed by left brain and carry task-relevant information (e.g., suggestions for solving problems, directions, questions about a task). This differentiated processing occurs without an actor's awareness.
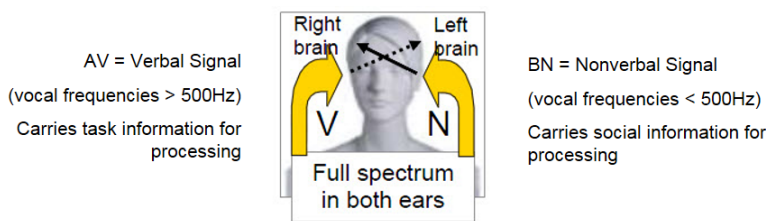

FIGURE 9

Vocal signal processing at different frequencies by different brain regions. Nonverbal signals occur at lower vocal frequencies (below 500Hz) and contain social information that enables group members to dynamically adjust to one another to manage social interaction. Verbal signals, in contrast, are discernible above the 500Hz level, and carry task-relevant information, including possible problem solutions, questions, directions for completing a task.

In an innovative strategy, Professor Dippong's team proposed that this process most likely evolves as a process of accommodation, in which actors seize status, in part by dominating the low frequency component of the voice spectrum. Also, however, other actors cede dominance as the interactions progress, leading to emergence of a distinctive status hierarchy in the group that can be operationalized and tracked over the course of group interaction. Additionally, Dippong hypothesized that when members move from one group to another, their vocal patterns shift, to the extent that their relative status in the new group changes vis-à-vis the prior group. That is, an individual may cede dominance of the low frequency spectrum in one group, but dominate it another. This hypothesis will be tested in an experiment in the coming year, offering new insights on how status

hierarchies emerge and change in groups as group membership changes, and the role that biophysiological processes may play in these dynamics. It also offers new ways to understand the formation and operation of group hierarchies and the role they play in leadership, influence, and decision-making.

C. Biophysiological and Social Predictors of Political Violence
Professor William Reed, University of Maryland, Single Investigator Award

Understanding factors that contribute to individual propensities for violence remains an ongoing concern of the security community. There has been considerable work on institutional and economic factors that may drive people toward violent rebellion, but why inequalities and repression drive some toward violence but not others remains a mystery. Professor William Reed proposes that the answer may be found in examining biophysiological factors. Specifically, his research aims to explore genetic variation in two genes, MAO-A and 5-HTT, which have been linked to aggression in adulthood that is correlated with early childhood trauma. Professor Reed is developing a sophisticated diathesis-stress model to hypothesize that a specific genetic vulnerability, in this case inefficiency in serotonin transportation resulting from low MAO-A/short 5-HTT alleles, when combined with an environmental stressor, such as repression, increases rates of particular behaviors, in this case violent aggression (see FIGURE 10). This approach promises to address past shortcomings in research on genetic determinants of social behavior that have failed to adequately account for environmental conditions that are critical to genetic expression. Moreover, it represents the first attempt to link gene x environment interactions to political violence.
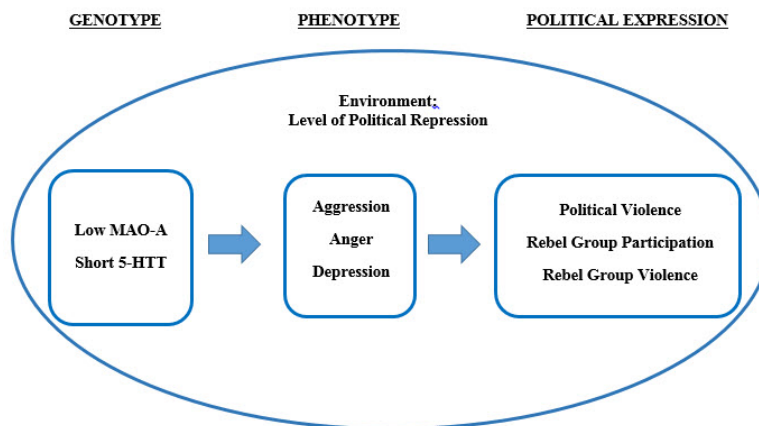

FIGURE 10

Causal model depicting path from genetic variation to engagement in violence. Research in political sciences has traditionally focused on the right box in the diagram, with challenges in explaining substantial individual variation in these behaviors. Integrating political science approaches with behavioral genetics offers a strategy for addressing this challenge.

Professor Reed is collecting genetic samples from a sample of combatants and non-combatants within particular social groups, along with survey data on past and current experiences with political repression, inequality, and forms of political participation. A matched sample of groups from other social collectives will be included to overcome a common issue in candidate gene association research in which focus on particular populations creates confounds in the findings. It is anticipated that in FY17, Professor Reed's laboratory will generate new insights on gene x environment interactions that will offer the potential to quell violence by predicting it before it emerges and developing interventions to address the environmental factors that spur violent responses.

D. Sensorimotor Function in Elite Athletes
Professor Lawrence Appelbaum, Duke University, Single Investigator Award

Highly experienced soldiers and athletes are experts at processing visual information and therefore developing an understanding of how their visual skills differ from others can inform models of learning while also uncovering the upper bounds of human ability. The goal of the proposed research is to perform secondary analysis of data collected through a large-scale sensory performance program that includes measures of vision,

cognition, and visual-motor control in hundreds of soldiers and thousands of athletes at all levels of achievement. Exploring variability in sensorimotor abilities over this large and unique population will help to uncover how visual skills relate to athletic and military expertise, real-world achievement, and resilience to traumatic brain injury. In recent years scientists have begun to make progress in understanding which aspects of sensorimotor function are enhanced in high achieving individuals, however, this research has been limited by small sample sizes, disparate tasks, and challenges in mapping laboratory experiments onto real-world outcomes. The present research project plans to overcome these limitations by making use of an existing performance program from academic and military partners of the Nike Sports Research Lab that has already collected data from thousands of soldiers and athletes at all levels of achievement. Professor Appelbaum's research will focus on analysis of past and future data collected with the Nike Sensory Station, a reliable and cross-validated computerized assessment device that measures nine sensorimotor skills. In FY16 Professor Appelbaum assembled and organized all the psychometric and demographic data, sports statistical data, and baseline concussion data from the large multi-center database of soldiers and athletes and conducted preliminary analyses (see FIGURE 11).
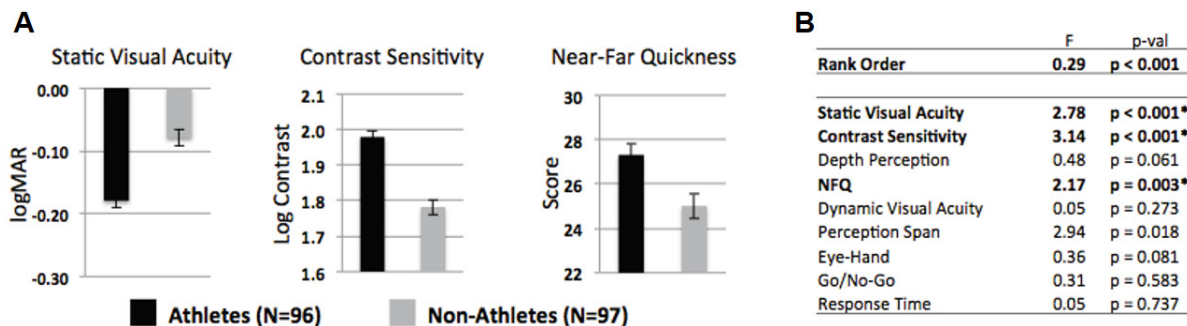

A

Static Visual Acuity | Contrast Sensitivity | Near-Far Quickness

Athletes (N=96)   Non-Athletes (N=97)

B

	F	p-val
Rank Order	0.29	$p < 0.001$
Static Visual Acuity	2.78	$p < 0.001*$
Contrast Sensitivity	3.14	$p < 0.001*$
Depth Perception	0.48	$p = 0.061$
NFQ	2.17	$p = 0.003*$
Dynamic Visual Acuity	0.05	$p = 0.273$
Perception Span	2.94	$p = 0.018$
Eye-Hand	0.36	$p = 0.081$
Go/No-Go	0.31	$p = 0.583$
Response Time	0.05	$p = 0.737$

FIGURE 11

Visual and cognitive differences exist between male collegiate athletes and male collegiate non-athletes. (A) Athletes performed significantly better on measures of static visual acuity (lower is better), contrast sensitivity, and near-far quickness. (B) Trending differences exist for perception span but do not reach Bonferroni adjusted alpha (0.0055).

In FY17 it is anticipated that Professor Appelbaum's team will determine if sensorimotor skills predict on-field performance. Using prospective analyses, he will test the hypothesis that sensorimotor skills are predictive of game statistics for specific on-field players in multiple sports, thereby advancing knowledge about what sensorimotor skills are valued for real-world success. He will also compare within and between specific military and sports cohorts to develop a detailed understanding of how different demands relate to better or worse sensorimotor skills. The present research offers a unique and cost-effective opportunity to explore the relationship between sensorimotor skills and expertise in a large sample of high-achieving soldiers and athletes.

E. Artificial Cells for Novel Synthetic Biology Chassis
Professor Neal Devaraj, University of California - San Diego, MURI Award

Mastering the capabilities of living systems is a scientific grand challenge that could catalyze the discovery, design, and synthesis of new materials. Biomimetic research has long aimed to create artificial cells consisting of minimal biochemical elements yet capable of performing functions with the extraordinary ability of naturally occurring cellular systems. An attractive route is to develop hybrid cells consisting of artificial supramolecular structures fully integrated with biological elements. Such artificial cells would be able to incorporate the toolbox of synthetic biology, such as genetic circuits and exquisitely evolved biochemical pathways, while possessing the stability, organization, and predictability of purely synthetic systems. A MURI team led by Professor Neal Devaraj is exploring the assembly of an artificial cell by integrating artificial growing chemical membranes with encapsulated dynamic gene networks and engineered molecular transport mechanisms to create hybrid "cells" capable of mimicking the function of natural cells but with improved control, stability, and simplicity. A novel research avenue was recently developed within this program that evolved from the team's efforts to incorporate pore-forming proteins into their artificial cells to allow supply of precursors to the "cells" and removal of reaction products. The team needed a model system in which membrane/shell porosity could be precisely

controlled without destabilizing the integrity of the "cell". They discovered that semipermeable polymeric capsules were an excellent model in that porosity could be easily controlled under a wide range of relevant parameters, they are very stable, and monodisperse populations can be rapidly produced. The development of these porous polymeric capsules led to the discovery that proteins produced within one capsule could diffuse into a neighboring capsule, akin to cell-cell communication in biological tissue systems.

It is anticipated that in FY17 the MURI team will re-create spatiotemporal patterning in a synthetic tissue of artificial cells using engineered genetic networks. The team plans to develop a method to array porous polymeric capsules containing DNA into large dense "tissues." These artificial tissues will be perfused with reagents for transcription and translation to create the far-from-equilibrium conditions necessary for dynamic pattern-forming regulatory networks to function. Finally, the team aims to design and implement genetic networks that generate spatiotemporal reaction diffusion patterns in the synthetic tissue. Individual polymeric capsules will produce transcription factors that diffuse through the tissue and interact in competing positive and negative feedback processes to generate spatiotemporal patterns such as waves, spirals, and Turing-like structures, which are apparent in a variety of biological systems, from embryonic development to structural coloration/camouflage in the animal kingdom (see FIGURE 12).
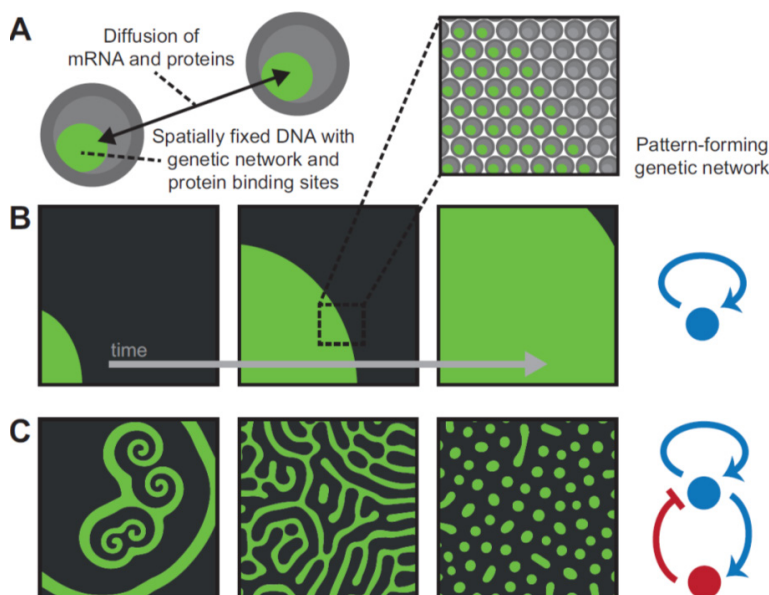

FIGURE 12

Artificial cells organized into a synthetic tissue. (A) Artificial cells in a synthetic tissue contain spatially fixed "genomes" encoding genetic networks and transcription factor binding sites. Protein products of the transcription-translation reaction diffuse from capsule to capsule through the tissue. (B) A positive feedback loop produces a trigger wave of reporter protein synthesis (green) that spreads through the tissue. (C) When negative feedback is added to the genetic network, more complex patterns form such as spirals of travelling waves (left) or stationary Turing patterns (middle, right). Patterns in C reproduced from Kondo and Miura, 2010.

The artificial cells to be developed through this effort will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology and supporting the development of DoD-relevant technologies including sense-and-respond systems, reactive coatings, and drug delivery platforms. A non-living synthetic biology chassis would also enable cost-effective production of high-value molecules that are toxic to living cells, including alternative fuels, novel biomaterials (e.g., non-natural sequence-defined polymers), cytotoxic molecules (e.g., antimicrobial agents, pharmaceuticals) or complex biological molecules (e.g., antibodies). The simplified model "tissue" that will be developed has potential to positively impact efforts related to tissue engineering. Recapitulating the patterning of biological tissues is a major challenge for regenerative medicine, as only properly organized tissues are functional.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Micheline Strand
Division Chief
Program Manager, Genetics

Dr. Stephanie McElhinny
Program Manager, Biochemistry

Dr. Frederick Gregory
Program Manager, Neurophysiology and Cognitive Neuroscience

Dr. Robert Kokoska
Program Manager, Microbiology

Dr. Lisa Troyer
Program Manager, Social and Behavioral Science

B. Directorate Scientists

Dr. Hugh De Long
Director (incoming), Physical Sciences Directorate

Dr. Douglas Kiserow
Director (outgoing), Physical Sciences Directorate

Dr. Peter Reynolds
Senior Scientist, Physical Sciences Directorate

Dr. J. Aura Gimm
Program Manager, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies

Dr. Kelby Kizer
Physical Scientist and Technical Assistant to the PSD Director

Mr. John McConville
Technology Transfer Officer, Institute for Soldier Nanotechnologies

C. Administrative Staff

Ms. Inez Kendall
Contract Support

Ms. Wanda Lawrence
Contract Support

CHAPTER 7: MATERIALS SCIENCE DIVISION

I.   OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2016* is to provide information on the programs and basic research supported by ARO in fiscal year 2016 (FY16), and ARO's mission to create basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Materials Science Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY16.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Materials Science Division seeks to realize improved material properties by embracing long-term, high risk, high-payoff opportunities for the U.S. Army, with special emphasis on four Program Areas: Materials by Design, Mechanical Behavior of Materials, Physical Properties of Materials, and Synthesis and Processing of Materials. The objective of research supported by the Materials Science Division is to discover the fundamental relationships that link chemical composition, microstructure, and processing history with the resultant material properties and behavior. These research areas involve the discovery of the fundamental processes and structures found in nature, as well as developing new materials, material processes, and properties that promise to significantly improve the performance, increase the reliability, or reduce the cost of future Army systems. Fundamental research that lays the foundation for the design and manufacture of multicomponent systems such as composites, hierarchical materials and "smart materials" is of particular interest. Other areas of interest include new approaches for materials processing, composite formulations, and surface treatments that minimize environmental impact. Finally, there is general interest by the Division in research to identify and fund basic research in manufacturing science, which will address fundamental issues related to the reliability and cost (including environmental) associated with the production and long-term operation of Army systems.

2. Potential Applications. Research managed by the Materials Science Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter and battle systems. In the long term, the basic research discoveries made by ARO-supported materials research is expected to provide a broad base of disruptive and paradigm-shifting capabilities to address Army needs. Advanced materials will improve mobility, armaments, communications, personnel protection, and logistics support in the future. New materials will target previously identified Army needs for stronger, lightweight, durable, reliable, and less expensive materials and will provide the basis for future Army systems and devices. Breakthroughs will come as the fundamental understanding necessary to achieve multi-scale design of materials, control and engineering of defects, and integration of materials are developed.

3. Coordination with Other Divisions and Agencies. To realize the vision of the Materials Science Division and maximize transition and leveraging of new materials discoveries worldwide, the Division collaborates with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), and across federal-funding agencies (*e.g.*, Nanoscale Science and Engineering Technology subcommittee, and in international forums (*e.g.*, the Technical Cooperation Program). The Materials Science Division is also very active in collaborating with other ARO Divisions to co-fund research, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. In particular, ongoing collaborations exist with the ARO Chemical Sciences, Electronics, Life Sciences, Mechanical Sciences, Mathematical Sciences, and Physics Divisions.

In addition, the Division's research portfolio will reveal previously unexplored avenues for new Army capabilities while also providing results to support (i) the Materials Research Campaign's goals to extend the state-of-the-art in materials design, mechanical behavior of materials, physical properties of materials, and synthesis and processing research. The Division also supports the Sciences for Lethality and Protection Campaign with extraordinary lightweight materials, force-activated materials, stabilized nanostructured materials, manufacturing process science, novel electronics, and advanced sensory materials. The Division also supports the Sciences for Maneuver Campaign with unique materials for advanced power storage and generation and lightweight structures, in addition to low-cost manufacturing and repair processes.

B. Program Areas

The Materials Science Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY16, the Division managed research within these five Program Areas: (i) Materials by Design, (ii) Mechanical Behavior of Materials, (iii) Physical Properties of Materials, (iv) Synthesis and Processing, and (v) Earth Materials and Processes. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Materials by Design. The Materials by Design Program Area seeks to establish the experimental techniques and theoretical foundations needed to facilitate the hierarchical design and bottom-up assembly of multifunctional materials that will enable the implementation of advanced materials concepts including transformational optics, biomimetics and smart materials. This Program Area is divided into two research Thrusts:

> (i) Directed 3D Self-Assembly of Materials is aimed at enabling the directed 3D assembly of reconfigurable materials, and developing viable approaches to the design and synthesis of multi-component materials incorporating hierarchical constructs.

> (ii) Functional Integration of Materials focuses on demonstrating the predictive design and integration of functional properties into complex multi-component systems, and developing analytical techniques for interrogating the evolution of the 3D structure and properties of material assemblies at the nanoscale.

2. Mechanical Behavior of Materials. The Mechanical Behavior of Materials Program Area seeks to reveal underlying design principles and exploit emerging force-activated phenomena in a wide range of advanced materials to demonstrate unprecedented mechanical properties and complementary behaviors. This Program Area is divided into two research Thrusts:

> (i) Force-Activated Materials involves demonstration and characterization of robust mechanochemically adaptive materials based on force-activated molecules and force-activated reactions, tailoring the deformation and failure mechanisms in materials to mitigate the propagation of intense stress-waves and control energy dissipation, and the creation of a new class of adaptive structural materials that demonstrate "mechanical homeostasis."

> (ii) Mechanical Complements in Materials discovers superior ionic transport materials and transparent materials through a complementary, interdependent, optimization of mechanical properties, catalyzes a self-sustaining investigation of fiber precursors, tailored for lateral and axial interactions, to generate new paradigms for revolutionary structural fibers, and discovers and validates new atomic-scale strengthening mechanisms governing bulk mechanical behavior.

3. Physical Properties of Materials. The Physical Properties of Materials Program Area seeks to elucidate fundamental mechanisms responsible for achieving extraordinary electronic, photonic/optical, magnetic and thermal properties in advanced materials to enable innovative future Army applications. This Program Area is divided into two research Thrusts:

> (i) Novel Functional Materials Thrust: This thrust supports the discovery of novel functional materials such as free-standing 2D materials/heterostructures/hybrids, Spin-Caloritronic materials, co-crystals, and other such materials with unique structures, compositions and properties. The thrust focus is on the synthesis,

modeling and novel characterization of these materials (organic/inorganic/hybrids) to determine unprecedented functional properties (semiconducting, superconducting, ferroelectric/multiferroic etc.).

(ii) Defect Science & Engineering thrust explores the basic research opportunities in design, control and advanced characterization of various defects (point, line, area, volume etc.) in functional materials and elucidates different mechanisms during thin film growth/bulk materials processing that influence the extraordinary physical properties of functional materials.

4. Synthesis and Processing of Materials. The Synthesis and Processing of Materials Program Area seeks to discover and illuminate the governing processing-microstructure-property relationships for optimal creation of superior structural and bulk nanostructured materials. This Program Area is divided into two research Thrusts:

(i) Stability of Nanostructured Materials focuses on the creation of thermally-stable, ultrahigh strength nano-crystalline materials through interfacial grain boundary engineering, and the realization of high strength, stable nanostructured alloys via pinning nano-precipitates and internal coherent boundaries.

(ii) Manufacturing Process Science supports discovery of the fundamental physical laws and phenomena of materials processes, and the exploitation of unique phenomena that occur under metastable and complex processing conditions for the creation of revolutionary materials.

5. Earth Materials and Processes. The Earth Materials and Processes Program Area seeks to elucidate the properties of natural and man-made Earth surfaces, with the goals of revealing their histories and governing dynamics and developing theory that describes physical processes responsible for shaping their features. This Program Area is closely coordinated with the Environmental Chemistry Program Area, within the Chemical Sciences Division. This Program Area is divided into two research Thrusts:

(i) Earth Surface Materials aims to utilize experiments, models, and theory development to describe the physical and mechanical properties and behaviors of rocks, minerals, and soil, and to exploit the properties of these materials to provide quantitative information on recent and ongoing surface processes and perturbations.

(ii) Surface Energy Balance aims to determine, at Army-relevant spatial and temporal scales, how natural and artificial surfaces (e.g., soil, sand, or concrete) store and conduct energy depending on their spatial relationships, inherent material properties, and imparted features such as moisture storage and evapotranspiration.

C. Research Investment

The total funds managed by the ARO Materials Science Division for FY16 were $36.7 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY16 ARO Core (BH57) program funding allotment for this Division was $6.0 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $5.1 million to projects managed by the Division. The Division also managed $19.3 million of Defense Advanced Research Projects Agency (DARPA) programs, $1.7 million of Congressional funding and $0.7 million provided by other Federal agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $2.0 million for contracts. In addition, $1.9 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $1.1 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY16 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY16 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY16, the Division awarded 26 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Ian Baker, Dartmouth College; *Synthesis and Processing of Materials: Directional Recrystallization Processing*
- Professor Laurent Bellaiche, University of Arkansas; *Discovering and Understanding Striking Phenomena in Dipolar Materials*
- Professor Raffi Budakian, University of Waterloo; *Nanometer Scale Magnetic Resonance Imaging of Electron and Nuclear Spins*
- Professor Leila Deravi, Northeastern University; *Molecular Contributions to Coloration in Cephalopod Chromatophores for Bio-inspired Photonic Systems*
- Professor Mark Forest, University of North Carolina - Chapel Hill; *A Network-Science-Integrated Feedback Loop for Design of Multifunctional Polymeric Rod-Like Nanocomposites*
- Professor Neil Gershenfeld, Massachusetts Institute of Technology (MIT); *Assembling Assemblers with Functional Digital Materials*
- Professor Peter Hammel, Ohio State University; *Foundations for Nanoscale Resolution Magnetic Resonance Studies of Spin Dynamics and Defect Properties in Diamond Nanostructures*
- Professor Patrick Hopkins, University of Virginia; *Ultrafast Thermal Transport Mechanisms at Organic/Inorganic Nanoscale Interfaces*
- Professor Heinrich Jaeger, University of Chicago; *Dynamic Jamming in Concentrated Particle Suspensions*
- Professor Enrique Lavernia, University of California - Irvine; *Nanostructured High Entropy Alloys*
- Professor Tengfei Luo, University of Notre Dame; *Hard-Soft Material Interfaces with Superior Thermal Transport Properties*
- Professor Maiken Mikkelsen, Duke University; *Reconfigurable Optical Properties in the Near-IR Enabled by Bottom-Up Assembly of Nanoengineered Materials*

- Professor Gracious Ngaile, North Carolina State University; *Novel Multi-Functional Hybrid Drawing Process*
- Professor Konstantin Novoselov, University of Manchester; *Quantum Devices Based on 2D Atomic Crystals and their Heterostructures*
- Professor Bart Raeymaekers, University of Utah; *Synthesis of Multi-Functional Materials with Tailored Properties Using Scalable Ultrasound Directed Self-Assembly and Additive Manufacturing*
- Professor Rishi Raj, University of Colorado - Boulder; *Phase Transformations in Ceramics and Related Materials, Far From Equilibrium, Under The Influence of an Electric Field*
- Professor Shriram Ramanathan, Purdue University; *Structural and Electrical Properties of Metastable Oxide Phases Created Under Extreme Oxygen Pressures*
- Professor Darrell Schlom, Cornell University; *Creating and Manipulating Exotic Spin-and Charge-Ordered Structures in Superlattices*
- Professor Kathleen Stebe, University of Pennsylvania; *Curvature Directed Assembly of Particles into Reconfigurable Structures at Fluid Interfaces*
- Professor Klaus van Benthem, University of California - Davis; *Tailoring of Ceramic Microstructures by Electric Field-Activated Grain Growth*
- Professor Christian Van de Walle, University of California - Santa Barbara; *The II-IV Nitrides Materials System as a Novel Design Space for Quantum Materials*
- Professor Haydn Wadley, University of Virginia; *Synthesis and Processing of Hierarchical Inverse Opal Cellular Materials*
- Professor Xudong Wang, University of Wisconsin - Madison; *Two-Dimensional Growth of Free-Standing Nanosheets and Heterostructures by Ionic Layer Epitaxy*
- Professor Manfred Wuttig, University of Maryland - College Park; *Charge Density Wave Stabilized Magnetoelastics*
- Professor Yan Xia, Stanford University; *Leverage of Molecular and Macromolecular Architectures for Mechanically Responsive Materials*
- Professor Jianshi Zhou, University of Texas at Austin; *Stabilization of BCS Superconductivity Near Room Temperature in Hydrides Under High Pressure and the Characterization with THz Spectroscopy*

2. Short Term Innovative Research (STIR) Program. In FY16, the Division awarded four new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Arash Yavari, University of Georgia Tech Research Corporation; *Nonlinear Elastodynamics Cloaking*
- Professor Semyon Vaynman, Northwestern University Evanston Campus; *HCP Mg Alloys Formable at Room Temperature*
- Professor Chih-Hao Chang, North Carolina State University; *Enhancing Optical Transmission of Multilayer Composites with Interfacial Nanostructures*
- Professor Madhu Menon, University of Kentucky; *Synthesizing New Functional 2D Semiconducting Solids*

3. Young Investigator Program (YIP). In FY16, the Division awarded one new YIP project to drive fundamental research in areas relevant to the current and future Army. The following PI and corresponding organization were recipients of the new-start YIP award.

- Professor Timothy Rupert, University of California - Irvine; *Using Complexions to Fabricate Bulk Nanocrystalline Metals with Enhanced Ductility*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY16 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *2015 Material Research Society Fall Meeting & Exhibit*; Boston, MA; 29 November – 4 December 2015

- *40th International Conference on Advanced Ceramics and Composites.*; Boston, MA; 24-29 January 2016
- *2016 Gordon Research Conference on Multifunctional Materials and Structures*; Ventura, CA; 31 January - 5 February 2016
- *Electric Field Assisted Sintering and Related Phenomena Far From Equilibrium Conference*; Tomar, Portugal; 6-11 March 2016
- *2016 Material Research Society Spring Meeting & Exhibit*; Phoenix, AZ; 28 March – 1 April 2016
- *2016 Gordon Research Seminar on Bioinspired Materials*; Les Diablerets, Switzerland; 4-5 June 2016
- *5th International Conference "Smart and Multifunctional Materials*, Structures and Systems; Perugia, Italy; 5-9 June 2016
- *2016 Gordon Research Conference on Multiferroic and Magnetoelectric Materials*; Lewiston, ME; 7-12 August 2016
- *Science Challenges in Low Temperature Plasma Science and Engineering: Enabling a Future Based on Electricity through Non-Equilibrium Plasma Chemistry*; Arlington, VA; 22-23 August 2016

5. Special Programs. In FY16, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded five new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES. These awards constitute a significant portion of the basic research programs managed by the Materials Science Division; therefore, all of the Division's active MURIs are described in this section.

1. Reconfigurable Matter from Programmable Colloids. This MURI began in FY10 and was granted to a team led by Professor Sharon Glotzer at the University of Michigan - Ann Arbor. This MURI project is co-managed by the Materials Science and the Chemical Sciences Divisions. The goal of this program is to enable the design and synthesis of an entirely new class of self-assembled, reconfigurable colloidal material capable of producing materials with radically increased complexity and functionality. This will revolutionize the ability to build complexity and functionality into materials in the future. Opportunities for manipulating the assembly process include the utilization of shape, intermolecular interactions, induced conformation changes, functionalized adduct and site-specific binding groups, molecule-to-substrate interactions, and external fields. Pathways including both sequential assembly and selective disassembly processes are being investigated. Selective disassembly and reconfigurability are to be accomplished by judicious exposure to heat, pH or light. The research includes aspects of self-limiting growth of superclusters. The experimental program is complemented by a very strong theoretical component. Research thrusts include:

- Sequential staged self-assembly of nano-particles into complex and hierarchical architectures
- Development of theoretical tools and computational algorithms to model the self-assembly process, to identify stable self-assembly pathways that lead to the targeted hierarchical structures, and finally to predict the final properties of the assembled material
- Future derivation of tailored properties and functions within highly complex or hierarchical materials

2. Stress-controlled Catalysis via Engineering Nanostructures. This MURI began in FY11 and was granted to a team led by Professor William Curtin at Brown University. The objective of this research is to prove that macroscopic applied loading can be used to actively control and tune catalytic reactions through the use of innovative nanoscale material systems.

This research is based on the hypothesis that active control using cyclically-applied stress can alleviate the well-established "volcano" effect wherein a desired reaction is optimal only in a narrow operating window due to competing reactions, and thereby overcome what has been believed to be a fundamental limiting factor in design of catalytic systems. The scientific underpinning will be demonstrated by developing two general platforms that

can sustain high mechanical loading while also accommodating a range of material systems and catalytic reactions. The main outcome of the project will be the unambiguous proof-of-principle that stress can be used to substantially modify and control chemical reactions, along with possible engineering paths, via both thin film and bulk metallic glass nanostructures for implementing stress control across a wide material space.

3. Atomic Layers of Nitrides, Oxides, and Sulfides (ALNOS). This MURI began in FY11 and was granted to a team led by Professor Pulickel Ajayan at Rice University. The main objective of this MURI is to explore innovative top-down and bottom-up routes for the synthesis or isolation of high quality uni-lamellar sheets and ribbons of nitrides, oxides, and sulfides and to characterization these free standing 2D atomic layers to establish structure-property correlations in 2D layers.

The synthetic approaches of this research will span from simple mechanical/chemical exfoliation techniques to controlled chemical vapor deposition to create various 2D freestanding materials. Researchers will use computational tools based on density functional theory (DFT) methods to investigate binding energies, barriers and stabilities of different dopants and how they affect the band structure of the 2D host materials. 2D materials will be characterized for electrical conductivity/resistivity, Hall effect, carrier concentration, mobilities, ionic conductivity and thermal conductivity. If successful, this project could advance the basic science required to develop future DoD applications in chemical and biological sensors, opto-electronics, and power and energy.

4. Translating Biochemical Pathways to Non-Cellular Environment. This MURI began in FY12 and was awarded to a team led by Professor Hao Yan at Arizona State University. This research program is being co-managed by the Life Sciences and Materials Science Divisions. This MURI is exploring how biochemical pathways can potentially function in a non-cellular environment. Cells provide a precisely organized environment to promote maximum efficiency of biochemical reaction pathways, with individual enzymatic components organized via multi-subunit complexes, targeted localization in membranes, or specific interactions with scaffold proteins. The eventual translation of these complex pathways to engineered systems will require the ability to control and organize the individual components outside of the natural cellular environment. Although biological molecules have been successfully attached to inorganic materials, this process often requires chemical modification of the molecule and can restrict its conformational freedom. An alternative approach to maintain biological activity outside of the cell, while preserving conformational freedom, is to encapsulate enzymes within specialized materials or structures. Unfortunately, surface patterning of current encapsulating agents has not achieved the precision required to replicate the organizational capabilities of the cell.

The objective of this research is to develop the scientific foundations needed to design, assemble, and analyze biochemical pathways translated to a non-cellular environment using 3D DNA nanostructures. The MURI team is using DNA nanostructures to direct the assembly of selected biochemical pathways in non-cellular environments. The focus of this research is to develop the scientific foundations needed to translate multienzyme biochemical reaction pathways from the cellular environment to non-biological materials. The ability to translate biochemical reaction pathways to non-cellular environments is critical for the successful implementation of these pathways in DoD-relevant technologies including responsive material systems, solar cells, sensor technologies, and biomanufacturing processes.

5. The Physics of Surface States with Interactions Mediated by Bulk Properties, Defects and Surface Chemistry. This MURI began in FY12 and was awarded to a team led by Prof Robert Cava of the Princeton University. This research is co-managed by the Physics and Materials Science Divisions. The objectives of this project are the discovery, growth, and fabrication of new materials that will display new topologically-stabilized electronic states in both 3D crystals and thin films grown by MBE. Those new materials will be characterized by many different methods including high resolution and spin resolved photoemission spectroscopy, transport, and STM measurements, X-ray scattering, and electron microscopy. The new materials of interest are particularly those that will display interactions arising from the presence of magnetism, such as those based on the heavy metal iridium, and interactions of topological states with superconductivity. State-of the- art materials science methods to optimize the properties of known topological insulators – in particular to enhance the interactions of the surface states with phenomena such as superconductivity are proposed. The correlation of the character of the chemically modified surfaces with the electronic properties will be performed. The team will address new frontiers in physics, such as proximity induced superconductivity in TIs, the 3D TI superconductor CuxBi2Se3, band bending surface capacitance and screening in TIs, and the giant Rashba effect in BiTeI etc.

6. Materials with Extraordinary Spin/Heat Coupling. This MURI began in FY13 and was granted to a team led by Professor Roberto Myers of the Ohio State University. The objectives of this project include understanding the structure-property relationships for coupling heat and spin current in various materials and synthesize magnetic materials with extraordinary and tunable thermal conductivity due to spins, understanding non-equilibrium phonon-magnon transport and the mechanisms behind Spin Seebeck Effect, and finally measuring and understanding phonon-magnon drag and phonon-electron drag in materials.

If successful, this project may lead to long-term applications such as temperature sensors, thermal spintronic devices, solid-state Spin Seebect Effect -based power generators, thermal management in electronic and vehicular applications, and tunable thermal conductivity in materials via magnetic field, microwaves, and light.

7. Theory and Experiment of Cocrystals: Principles, Synthesis and Properties. This MURI began in FY13 and was awarded to a team led by Professor Adam Matzger of the University of Michigan at Ann Arbor. This MURI team is investigating molecular co-crystal formation and the implications for controlling solid-state behavior. This research is co-managed by the Chemical Sciences and Materials Science Divisions.

The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Co-crystallization has the potential to impact the macro-scale performance of many materials, ranging from energetic materials, to pharmaceuticals, to non-linear optics. Unfortunately, the dynamics of molecular co-crystal formation is poorly understood. Molecular co-crystals contain two or more neutral molecular components that rely on non-covalent interactions to form a regular arrangement in the solid state. Co-crystals are a unique form of matter, and are not simply the result of mixing two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure 'parent' crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has not been exploited in broader chemistry and materials science research areas. A recent breakthrough discovery demonstrates that co-crystallization can be used to generate novel solid forms of energetic materials.

The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and to use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties. In the long term, a better understanding and control of molecular co-crystallization has the potential to improve the properties of a variety of materials, including: energetic materials, pharmaceuticals, organic semiconductors, ferroelectrics, and non-linear optical materials.

8. Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials. This MURI began in FY14 and was awarded to a team led by Prof Luskin, Mitchell of the University of Minnesota. This research is co-managed by the Mathematics and Materials Science Divisions. The objective of this project is to develop efficient and reliable multiscale methods to couple atomistic scales to the mesoscopic and the macroscopic continuum for layered heterostructures. Layered heterostructures represent a dynamic new field of research that has emerged from recent advances in producing single atomic layers of semi-metals (graphene), insulators (boron nitride) and semiconductors (transition metal dichalcogenides). Combining the properties of these layers opens almost unlimited possibilities for novel devices with desirable, tailor-made electronic, optical, magnetic, thermal and mechanical properties. The vast range of possible choices requires theoretical and computational guidance of experimental searches; experimental discovery can in turn inform, refine and constrain the theoretical predictions.

The proposed research will develop efficient and reliable strongly-linked multiscale methods for coupling several scales based on a rigorous mathematical basis. Specifically: 1) The rigorous coupling of quantum to molecular mechanics will be achieved by properly taking into account the mathematics of aperiodic layered structures. 2) The coupling of atomistic-to-continuum will be achieved by methods that can reach the length scales necessary to include long-range elastic effects while accurately resolving defect cores. 3) New accelerated hybrid molecular simulation methods, specially tailored for the weakly interacting van der Waals heterostructures, will be developed that can reach the time scales necessary for synthesis and processing by CVD and MBE. 4) The simulations will be linked to macro and electromagnetic modelling to understand the physics and bridge to experimental investigation.

The challenge of modeling layered heterostructures will promote the development of strongly-linked multiscale models capable of handling many other materials systems with varied applications, including composites, meta-atoms (atomically engineered structures), and bio-materials that are of interest to the Army.

9. Advanced 2-Dimensional (2D) Organic Networks. This MURI began in FY16 and was granted to a team led by Prof. William Dichtel at Cornell University. The objective of this research is to create stable, free-standing, single-monomer-thick 2D crystalline organic polymer nanosheets/covalent organic frameworks (COFs) with designed electronic (conductivity, mobility, charge storage), optical (resonances, nonlinearities), and structural properties.

The team will combine mechanistic studies, theory, microscopy, and spectroscopy to gain fundamental insight into the 2D polymerization processes. Specifically the team will address the challenges in 2D COF synthesis and characterization by focusing on the following three major research thrusts: (1) exploration of nucleation, bond exchange, and polymerization of 2D COFs to improve their long-range order and morphological form and isolate 2D COFs as single crystals; (2) investigation of new conjugated linkage chemistries, topologies, and doping strategies to impart extensive electronic delocalization and useful optical and electronic properties; and (3) fabrication of new hybrid device heterostructures based on the interfacing of 2D COFs with newly emerging 2D inorganic materials such as transition metal dichalcogenides.

10. Specifically Triggerable Multi-Scale Responses in Organized Assemblies MURI. This MURI began in FY16 and was awarded to a team led by Prof Sankaran Thayumanavan of the University of Massachusetts – Amherst and is being jointly managed by the Materials Science and the Chemical Sciences Divisions. The goal of this effort is to develop a fundamental understanding of how a molecular level detection event can be amplified and then propagated across a macroscopic material to affect a global property change that spans multiple length and time scales. Fundamental approaches for converting single event triggers into extended material responses based on liquid crystal reorientation, regulated amphiphile assembly, gel-to-sol depolymerization and release reactions, and protein-induced transformations are being investigated. A variety of trigger mechanisms based on pH, temperature, redox, light, and enzymatic release are to be developed. A key aspect of this effort is the real-time monitoring of the dynamic changes associated with the cooperative reorganization processes combined with a strong theoretical component aimed at developing models of the material responses and corresponding phase behavior. The breadth of this effort allows for objectives to be pursued in parallel to achieve a fundamental understanding of multi-scale signal propagation and amplification in hierarchical systems and the development of rational design principles for fabricating dynamically responsive material systems.

11. Quantum Materials by Design with Electromagnetic Excitation. This MURI began in FY16 and was awarded to a team led by Prof David Hsieh of Caltech and is being jointly managed by the Physics and Materials Science Divisions. The objective of the project is to create new electronic states of matter that are unobtainable through conventional solid-state synthesis. The team proposes to employ excitations across the entire electromagnetic (EM) spectrum, including with extremely high pulsed fields, to design, realize, and manipulate new phases and responses in strongly correlated materials. Specifically, the team will focus on realizing new correlated states via the following approaches, (1) EM stimulated, bond selective, tuning of charge hopping parameters, (2) direct EM modification of magnetic exchange, order, and frustration, (3) continuous EM control of dimensionality and hybridization, and (4) EM excitation across kinetic barriers to realize metastable states that are thermodynamically inaccessible. Using these non-equilibrium methods, they will aim at realizing some of the most sought-after phenomena in condensed matter physics including collective charge/current ordered phases, bandwidth controlled metal to Mott insulator transitions, quantum disordered magnets such as valence bond solids and highly entangled quantum spin liquid states, and low dimensional and quantum critical electron liquids with no quasiparticle description.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY16, the Division managed two new-start SBIR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase II contracts. These new-start contracts aim to bridge fundamental discoveries

with potential applications. A list of SBIR topics published in FY14 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY16, the Division managed three new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of three Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY14 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY16, the Division managed one new ARO (Core) HBCU/MI project and four new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The following PECASE recipients, previously nominated by this Division, were announced in this fiscal year by the White House. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Synthesis and Fundamental Studies of Atomic Layers, Atomic Quilts, and van der Waals Heterostructures. The objective of this PECASE, led by Professor Deji Akinwande at the University of Texas at Austin, TX is to synthesize novel free-standing two-dimensional (2D) atomic layers, atomic quilts of dissimilar 2D materials, and Van der Waal heterostructures of 2D materials and explore unique electronic, optical, and thermal properties of these novel structures. The PI proposes to synthesize homogeneous monolayers of several crystalline materials such as silicene, transition metal di-chalcogenides, hBN etc. using various processing routes. He proposed to employ a new route for silicene synthesis based on catalytic chemical vapor deposition using silane as a precursor. He also proposes to grow novel single-crystal epitaxial tetragonal mono and few layers of rare-earth pnictides to determine possible changes in semimetal to semiconducting transitions due to dimensional effects in these materials. He will also grow and characterize atomic quilts or mosaics of random or ordered patterns of dissimilar novel 2D materials. He will integrate 2D sheets and 1D nanoribbons which would afford bottoms-up multifunctional designer materials with tailored properties. A cross-cutting characterization integrating advanced microscopy, spectroscopy, and transport studies will be intimately inter-woven into the aforementioned research thrusts to elucidate physical properties of these materials/structures.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY16, the Division managed five new DURIP projects, totaling $1.1 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Nanostructured Materials for Power (NMP) Program

The DARPA NMP program seeks to exploit advanced nano-structured materials for revolutionary improvements in power applications of DoD interest. The ability to decouple and independently control physical, chemical, electromagnetic, and thermal phenomena through nanoscale design, is being tapped to enable improvements in the energy product of permanent magnets and the efficiency of future thermoelectric devices. The Materials Science Division currently co-manages projects within this program. The goals of these projects are ultimately to provide new nano-structured magnetic and thermoelectric materials with enhanced figures of merit for development of higher performance compact power sources in the future.

I. DARPA LoCo Program

The goal of the Local Control of Materials Synthesis (LoCo) program is to develop a low-temperature process for the deposition of thin films whose current minimum processing temperature exceeds the maximum temperature substrates of interest can withstand (e.g., chemical vapor deposited diamond on polymers). The Division currently co-manages projects within this program seeking to realize chemical and physical processes to meet the energetic/chemical requirements of thin film deposition (e.g., reactant flux, surface mobility, reaction energy, etc.), without reliance on broadband temperature input used in state-of-the-art chemical vapor deposition.

J. DARPA Low-Cost Light Weight Portable Photovoltaics (PoP) Program

The goal of the DARPA PoP program is to provide low-cost light-weight portable photovoltaics to DoD. The Materials Science Division currently co-manages projects within this program with the goal of exploring new materials solutions that can meet these goals.

K. DARPA Manufacturing Experimentation and Outreach (MENTOR2) Program

The DARPA MENTOR2 Program seeks to enhance defense readiness by improving both the training and the tools available to those who will be called on to utilize, maintain, and adapt high-technology systems in low-technology environments. MENTOR2 will pursue this goal by developing and demonstrating new training tools, new materials, and new manufacturing technologies in the fields of electromechanical design and manufacturing. It is envisioned that project based curricula employing MENTOR2 design and prototyping tools will teach a deeper understanding of high-technology systems and better enable future competence in the maintenance and adaptation of such systems through the manufacture of as-designed components or the design and manufacture of new components. The Division currently co-manages projects within this program seeking to explore the integration of materials manufacturing and learning approaches to develop and demonstrate new approaches to electromechanical design.

L. DARPA Fracture Putty Program

The DARPA Fracture Putty program seeks to create a dynamic putty-like material which, when packed in/around a compound bone fracture, provides full load-bearing capabilities within days, creates an osteoconductive bone-like internal structure, and degrades over time to harmless by-products that can be reabsorbed as the normal bone regenerates. This new material could rapidly restore a patient to ambulatory function while normal healing ensues, with dramatically reduced rehabilitation time and elimination of infection and secondary fractures. The Division currently co-manages projects within this program attempting to achieve a convergence of materials science, mechanics, and orthopedics to enable new paradigms in bone stabilization, growth, and regeneration.

M. DARPA Structural Logic Program

The DARPA Structural Logic program seeks to enable structural systems that make up the basis for modern military platforms and buildings to adapt to varying loads and simultaneously exhibit both high stiffness and high damping. By demonstrating the ability to combine stiffness, damping, and adaptive dynamic range in a single structure, the Structural Logic program will enable the design of military platforms with the ability to

continually change their properties to match the demands of a broad range of dynamic environments. The Division currently co-manages projects within this program seeking to realize novel design paradigms for passively adaptive structural systems that combine high stiffness, damping, and unprecedented adaptability.

N. DARPA Maximum Mobility and Manipulation Program

The DARPA Maximum Mobility and Manipulation program seeks to create and demonstrate significant scientific and engineering advances in robotics that will create a significantly improved scientific framework for the rapid design and fabrication of robot systems and greatly enhance robot mobility and manipulation in natural environments. Additionally, the program seeks to significantly improve robot capabilities through fundamentally new approaches to the engineering of better design tools, fabrication methods, and control algorithms. The Maximum Mobility and Manipulation program covers scientific advancement across four tracks: design tools, fabrication methodologies, control methods, and technology demonstration prototypes. The Division currently co-manages projects within this program seeking to realize novel material design and fabrication paradigms for advanced sensing and actuation materials.

O. DARPA Microphysiological Systems Program

The DARPA Microphysiological Systems program seeks to develop a platform that uses engineered human tissue to mimic human physiological systems. The interactions that candidate drugs and vaccines have with these mimics will accurately predict the safety and effectiveness that the countermeasures would have if administered to humans. As a result, only safe and effective countermeasures will be fully developed for potential use in clinical trials while ineffective or toxic ones will be rejected early in the development process. The resulting platform should increase the quality and potentially the number of novel therapies that move through the pipeline and into clinical care. The Division currently co-manages projects within this program seeking to realize safe and effective countermeasures based upon novel characterization tools, molecular structures, and materials architectures.

P. High Energy Laser Research & Development for HEL-JTO

The High Energy Laser Research & Development Program seeks to support farsighted, high payoff scientific studies leading to advances in HEL science and technology science with the end goal of making HELs lightweight, affordable, supportable, and effective on the modern battlefield. The Division currently manages solid-state laser research of processes and technologies that provide enhancement to the manufacturability of current and innovative design of ceramic gain material.

Q. DARPA Materials for Transduction (MATRIX), DSO-DARPA

Transducer materials convert energy from one form to another, such as thermal to electrical energy, or electric field to magnetic field. While significant progress has been made in advancing energy transducing material performance (e.g. thermoelectrics, multiferroics and phase changing materials) for certain applications, gains at the material level have not always translated into new devices and DoD capabilities. The goal of the MATRIX program is to extend materials breakthroughs to the device and systems level by integrating diverse modeling, design and fabrication communities in a unified research and development effort that bridges the material and the device domains. A major program thrust is the development of multiscale, multimodal design and engineering tools that have the potential to accelerate adoption of MATRIX technology into DoD platforms. The Division currently manages five programs within this DARPA Program:

- Solid State (Gyrator) Device for Low Power Electronics; Dwight Viehland, Virginia Tech.
- Phase-Change Materials Enabling Hyperspectral Imaging: Jeong Moon, HRL
- Wireless Cooling with Caloric Materials: Amy Duwel, Draper Labs
- Tunable Energy Efficient Multiferroic-based Electronics: Shashank Priya, Virginia Tech
- Integrated Magnetoelectric Devices: Carmine Vittoria, Northeastern University

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Materials Science Division.

A. Thermodynamics and Kinetics of Phase Changes in Layered Materials
Professors Evan Reed and Eric Pop, Stanford University, Single Investigator Award

The objective of this research is to investigate basic mechanisms of phase transformations (thermodynamics and kinetics of polymorphism) in 2D materials near ambient conditions. This will be accomplished by using a combination of DFT-based approaches, combined with cluster expansions for alloys and barrier calculations for kinetics. The research team has discovered a new physical mechanism through which the structural phase transition can be controlled in a 2D material. By developing DFT-based calculation approaches, they have predicted that the addition or removal of charge via electrostatic gating can induce a structural phase transition in the two-dimensional material $MoTe_2$ (see FIGURE 1). This new physical mechanism is distinct from the thermal and optical mechanisms that are commonly used in bulk phase-change materials, and is expected to be an effect that is observable only in a two-dimensional material. This mechanism is readily integrated into electronic devices, and holds potential for future nonvolatile information storage applications. The energy consumed in changing the phase of the material has the potential to be significantly lower than the thermal mechanisms currently employed in electronic devices because the energy is not lost due to diffusion of heat out of the material.
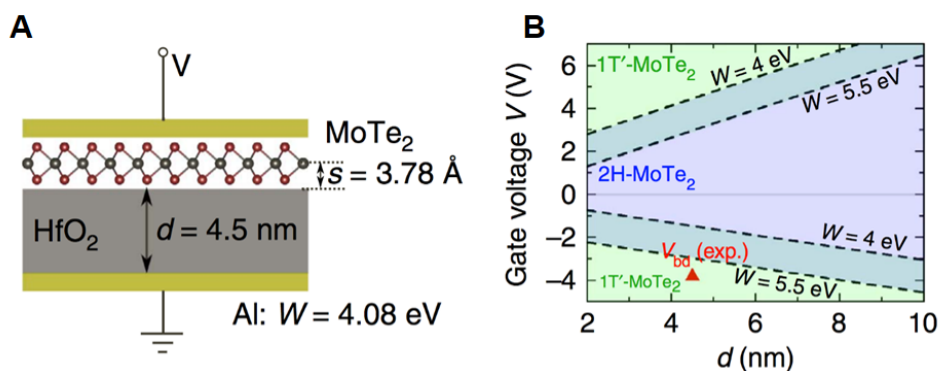

FIGURE 1

DFT-based calculation of 2D material phase transitions. The research team completed calculations of the addition or removal of charge via electrostatic gating can induce a structural phase transition in the 2D material $MoTe_2$. (A) Schematic of a single layer of $MoTe_2$ electrostatically gated using an oxide dielectric of thickness d. (B) Calculations of the voltage required to induce the H to T' structural change in $MoTe_2$ as a function of oxide layer thickness, suggesting experimentally achievable values of 1-4 V.

B. Creation of Spin Voltages in Magnetic Thin Films upon Exposure to Light
Professor Mingzhong Wu, Colorado State University, Single Investigator Award

The objective of this research is to understand the photon-electron-magnon interactions for the possible creation of spin voltages in magnetic thin films. The PI demonstrated for the first time that a spin voltage can be created by photons in a non-magnetic metal that is in close proximity to a magnetic insulator, a photo-spin-voltaic (PSV) effect (see FIGURE 2). Integral experimental and theoretical studies were carried out to understand underlying physical mechanisms of the PSV effect. The experiments included processing of several non-magnetic metal (NM) and magnetic insulator (MI) bi-layered structures. The PI conducted various experiments to understand the photon-driven electron excitation process, spin voltage establishment, and investigated materials with a strong PSV effect. The research team observed the PSV effect in NM/MI samples consisting of different NM layers including Pt, Pd, and Cr and different MI layers including a 23-nm-thick $Y_3Fe_5O_{12}$ (YIG) film, a 4.9-μm-thick YIG film, a 78-μm-thick doped YIG film, and a 1.2-μm-thick $BaFe_{12}O_{19}$ (BaM) film. Using different light

illumination configurations and various light sources and optical filters, they found that the effect is not attributed to any temperature gradient-associated effects or magnon excitations in the MI layer, but is due to photon-driven, spin-dependent electron excitations in the NM atoms in close proximity to the MI layer.
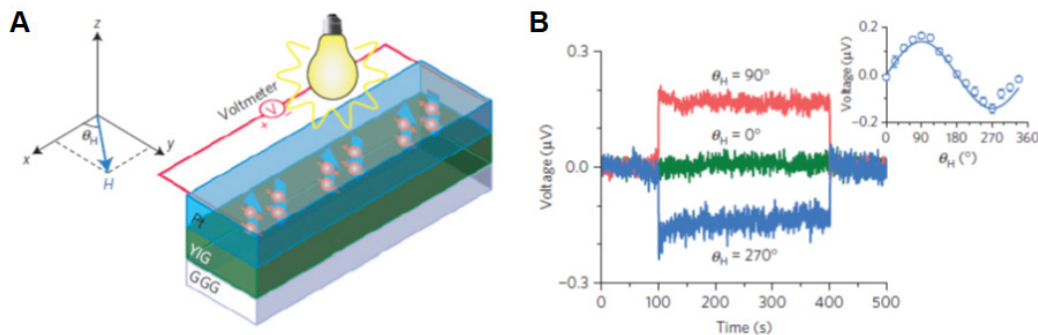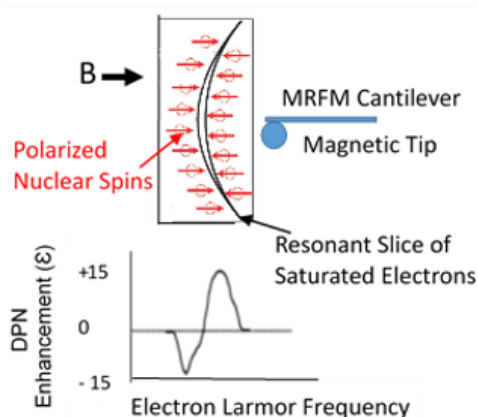

FIGURE 2

Main features of the PSV effect. (**A**) Experimental configuration to demonstrate the PSV effect. (**B**) Voltage signals measured for different field angles (θH) in response to light that was first turned on at 100 s and then turned off at 400 s. The inset shows the voltage as a function of θH.

C. Dynamic Nuclear Polarization Realized in a Magnetic Resonance Force Microscopy Experiment
Professor John Marohn, Cornell University, Single Investigator Award

The goal of this research is to improve on the spatial resolution of Magnetic Resonance Force Microscopy (MRFM) through the implementation of dynamic nuclear polarization techniques. A Cornell research team headed by Professor John Marohn report that they have achieved enhanced nuclear magnetization in a MRFM experiment conducted at 0.6 tesla and 4.2 kelvin by utilizing dynamic nuclear polarization (DNP) techniques. In these experiments a microwire coplanar waveguide delivered radio waves used to excite nuclear spins and microwaves to excite electron spins in a 250 nm thick nitroxide-doped polystyrene sample. Both electron and proton spin resonance were observed as a change in the mechanical resonance frequency of a nearby cantilever with an attached micron-sized nickel tip. The nuclear magnetic resonance (NMR) signal, not observed in conventional Curie-law magnetization measurements at 0.6 T, became observable when microwave irradiation was applied to saturate the electron spins. The resulting NMR signal's increased strength, buildup time, and dependence on microwave power and irradiation frequency was consistent with a transfer of magnetization from electron spins to nuclear spins. Due to the presence of the large magnetic field gradient introduced by the cantilever's magnetic tip, the electron spins in the sample were saturated only in a narrow microwave-resonant slice a mere 10's of nm thick. The spatial distribution of the nuclear polarization enhancement factor (ε) was mapped by varying the frequency of the applied radio waves (see FIGURE 3). The observed enhancement factor was zero for spins in the center of the resonant slice, $\varepsilon = +15$ (± 5) for nuclear spins proximal to the magnet, and $\varepsilon = -15$ (± 5) for spins distal to the magnet. This bipolar nuclear magnetization profile was consistent with cross-effect DNP in a 105 T/m magnetic field gradient. Although the observed DNP was relatively small, approximately 2 % polarization efficiency, it was the first time that it was ever measured in the presence of the large magnetic field gradient that is critical for conducting high spatial resolution NMR measurements. This accomplishment represents a major advance in the realization of a single-spin magnetic resonance imaging capability that would transform the study of molecular structures, biological processes and functional nanostructures.
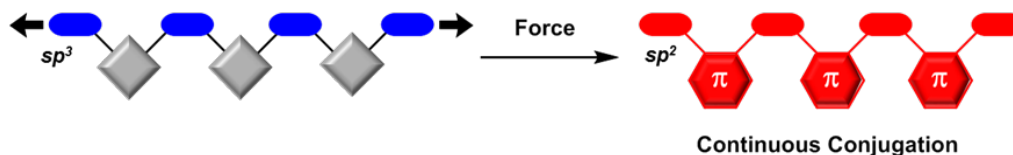
FIGURE 3

Schematic mapping of the spatial distribution of enhanced nuclear polarization showing positive Ɛ for spins proximal to the magnetic tip and negative Ɛ for distal spins.

D. Polymechanophores to Form Conjugated Molecular Structures
Professor Yan Xia, Stanford University, Single Investigator Award

The objective of this research effort is to explore the fundamental aspects for force-activation of functional groups and their coupling to the macroscopic matrices. The research has focused on discovering new mechanophores that give optical and chemical response to mechanical force. Work includes synthesizing a range of strained compounds and heterocycles synthesized from cycloaddition reactions, force coupling in complex macromolecular and network architectures, and absorption and fluorescence based assays to monitor the mechanochemical events in situ. In FY16, the work has evaluated two major classes of motifs, heterocycles and strained cyclic compounds, as potential mechanophores using sonication-based assay. Among the six novel chemical structures investigated, the first ever strained non-conjugated ladder structure (i.e., ladderene) was fabricated that unzips to form conjugated oligoenes in response to sonication (see FIGURE 4). This new mechanophore opens up a potential opportunity to convert an insulating polymer to a conjugated polyacetylene, which is unprecedented in both mechanochemistry and force-responsive materials. The result also constitutes the first example that a mechanophore can be directly polymerized to high MW to form a "polymechanophore.".

FIGURE 4

Continuous (domino-type) and efficient mechanochemical conversion of sp3 carbons to sp2 carbons to establish significant conjugation

E. 4D Characterization of Precipitate Formation and Evolution in Al-Cu Alloy
Professor Nikhilesh Chawla, Arizona State University - Tempe, Single Investigator Award

The dislocation/particle interactions that cause precipitate strengthening are governed by the precipitate's shape, size, and interface with the matrix. Precipitate formation and evolution occurs in three dimensions, but has been studied primarily by two-dimensional microscopy methods. In FY16 a team of researchers at Arizona State University succeeded in using the Advanced Photon Source at Argonne National Laboratory to perform Transmission X-ray Microscopy (TXM) on an Al-Cu 4wt% alloy. The TXM contained a hot stage that allowed the sample to be aged at 350 to 400°C in the chamber. The TXM beam scanned a series of 2D sections from a micropillar that were subsequently reconstructed into a 3D rendering that depicted the evolution of the microstructure as the aging progressed, depicting the growth, distribution, and orientation of the precipitate formation in the three spatial dimensions over time (see FIGURE 5). This effort was the first time ever the three-

dimensional precipitate network for this alloy was characterized in-situ. This work established an experimental method capable of testing theories regarding precipitate formation and microstructural coarsening. It also provides a means of measuring difficult to quantify, but important, factors such as diffusional coefficients, particle orientation and surface area, and precipitate distribution. The experimental data obtained from the TXM characterization is currently being utilized in computational simulations to enable advances in the processing and engineering of precipitate strengthened alloys.
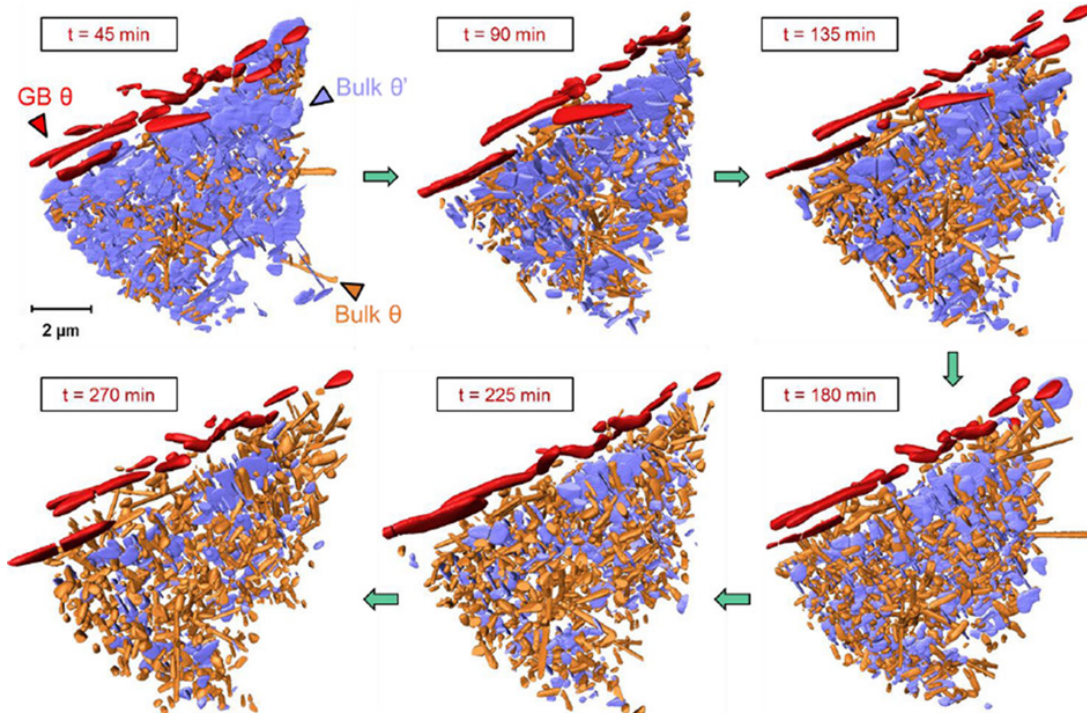

FIGURE 5
4D Microstructural characterization of an Al-Cu 4wt% alloy aged at 350°C

IV.   TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Surface Monitoring for Composition Control during Synthesis of Compound Semiconductor Films
Investigator: Philip Staib, Staib Instruments Inc. STTR Phase I & II
Recipients: ARL-SEDD

The objective of this research is to develop and test a powerful and innovative analysis technique to monitor and measure elemental composition of samples in situ & in real time with composition control feedback designed for all major commercial thin film growth chambers. The research team in collaboration with S&Es at ARL- SEDD has demonstrated a Real Time Elemental Monitoring System (rt-EMS) using a unique Auger Probe providing unprecedented instantaneous measurements for all elements on the surfaces using a unique Auger spectrometer, plus automated data acquisition and processing. This tool can be used to gain new insights to the evolution of the growth & chemical processes occurring at the interfaces. This real time information can be used to optimize material quality, reduce the production time/costs as well as in conducting basic research during advanced materials growth. This tool was tested during the growth of several advanced materials such as GaAsSb and GaN by molecular beam epitaxy at ARL-SEDD before making it available for commercial use.

B. Tunable Energy Efficient Electronics
Investigator: Professor Shashank Priya, Virginia Polytechnic Institute, Single Investigator Award
Recipient: AVX Corporation and United Technologies Research Center

Recent breakthroughs in co-fired ceramic laminate processing, compositional grading and low temperature grain texturing at Virginia Polytechnic Institute are now being transitioned to AVX Corporation and United Technologies Research Center under the DARPA MATRIX program. The goal of the program is to realize a new class of dynamically tunable passive electrical components (including capacitors, inductors and transformers), based on the incorporation of voltage-tunable magnetoelectric thin-film heterostructures. It is anticipated that this technology will lead to a new generation of DoD power conversion systems with significantly improved cost, size, weight and efficiency metrics. The transition partners in this effort include AVX Corporation, a multilayer ceramic components manufacturer, and United Technologies Research Center, a DoD prime contractor of high power conversion electronic systems for fighter aircraft. For demonstration purposes, individual tunable passive components and an integrated a dc-dc power converter are being designed and built to show how the integration of voltage tunable components (filters, LLC converters and point-of-load converters) can lead to higher system efficiencies and greatly improved SWAP performance.

C. 3D Printed Flexible Electronics
Investigator: Professor Jennifer Lewis, Harvard University, Single Investigator Award
Recipient: Lawrence Livermore National Laboratory and Air Force Research Laboratory

The objective of this research effort is to fabricate temporally and spatially patterned gels and nanocomposites that undergo dramatic changes in chemo-mechanical properties in response to external stimuli. More specifically, the aim is to lay the foundation for the field of four-dimensional printing by establishing robust control of not only the spatial dimensions of the sample, but also the time-dependent behavior of the system and hence, to enable patterning in space and time. In FY16, joint research efforts were initiated with the additive manufacturing teams at LLNL and AFRL to optimize print heads to target and optimize material properties. The collaborations have identified novel materials and robust processing strategies to enable soft sensors and flexible electronics.

D. Ballistic Evaluation of Ultrafine Grained Tungsten Alloy
Investigator: Professor Christopher Schuh- MIT, Boston Single Investigator Award
Recipients: U.S Army Armament Research Development Engineering Center (ARDEC)

This research has focused on the development of thermally stable nano-crystalline materials and has led to the successful fabrication of several nano-grained alloys at MIT. MIT provided projectiles fabricated from one of their W based nanocrystalline alloys to the Army Research Laboratory and Picatinny Arsenal for testing as a high performance penetrator. There were two aspects to the ballistic testing. The first was to evaluate the performance of the ultra-fine grained W-alloy as a penetrator; a more conventional cemented tungsten carbide penetrator was also tested for comparison purposes. The second goal was to explore whether the Forrestal equations used for evaluating long penetrators could be successfully applied to smaller caliber threats. MIT fabricated a W-8at%Cr-4at%Fe ultrafine grained alloy by mechanically alloying the powder mixture and consolidating using spark plasma sintering. Projectiles fashioned using both materials were fired out of a 5.56mm barrel into a cured concrete target. It was found that the Forrestal equations strongly correlated with the ballistic performance of the smaller scale projectiles, indicating that this framework can potentially be applied to smaller caliber threats. In terms of performance, the ultrafine W alloy was comparable to the cemented carbide. Based on its measured compressive strength, the ultrafine W alloy is potentially capable of much greater penetration than a comparably sized high strength steel round. These results were published in a communication in the International Journal of Impact Engineering.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Investigation of Dynamic Phenomena in Atomically Thin Layered Materials
Professor Chenggang Tao, Virginia Tech, Single Investigator Award

The objective of this research is to develop fundamental understanding of the mechanisms governing dynamic processes in two-dimensional (2D) materials. The PI will investigate novel thermodynamic phenomena in atomically thin layered materials, and further study the interplay between local structures, dynamic behaviors and external fields (e.g., electrical field). He proposes to use a unique combination of scanning tunneling microscopy and Q-plus atomic force microscopy to investigate the dynamic phenomena in 2D materials. It is anticipated that in FY17 the research team will investigate atomically thin transition metal di-chalcogenides (TMDs) such as MoS_2, $TiSe_2$, TaS_2 and WS_2 on various substrates.   Dynamic phenomena such as unique edge states of MoS2, charge density waves in $TiSe_2$ and vacancy island growth in TMD monolayers induced by a vertical electrical fields will be investigated. Results of this study can shed light on fundamental processes such as mass transport, growth, site-specific heterogeneous catalysis, and gas sensing.

B. Oxide-based Solid State Cooling
Professor Lane Martin, University of California – Berkeley, PECASE Award

The objective of this is to explore new approaches to solid state cooling. Researchers at Berkeley are conducting investigations on the physical mechanisms and related thermodynamics that underlies thermo-electrical responses (primarily pyroelectric and electrocaloric) in complex oxide materials. It is anticipated that in FY17, the research team will identify the key materials properties that control the temperature- and field-dependent entropic changes that occur in multiferroic/magnetoelectric heterostructures and in frustrated ferroelectric systems. If sucessful, first generation, solid-state-cooling devices will be fabricated and characterized for potential operation down to ~70K.

C. Nonlinear and Linear Elastodynamics Transformation Cloaking
Professor Arash Yavari, Georgia Institute of Technology, Single Investigator Award

The objective of this research effort is to explore and create a precise formulation of nonlinear and linearized elastodynamics cloaking. The combined approach seeks to develop a rigorous formulation of the cloaking problem in elastodynamics, including nonlinear and linearized elasticity under referential diffeomorphisms. In FY17, the research will seek to prove that transformation cloaking is possible for linear elasticity and to formulate the problem of cloaking of elastic waves in both nonlinear and linear elastodynamics.

D. Stress states in Fe-Cr Nanocrystalline Alloys
Professor Gregory Thompson, University of Alabama, Tuscaloosa- Single Investigator Award

The objective of this research is to understand the fundamental mechanisms governing compositional segregation in alloys by studying the stresses induced in thin films. It is anticipated that in FY17 the explanation will be found as to why Cr alloying in Fe thin films refines grain structures without impacting the stress state. This result, obtained in early FY16, was in contrast to experiments in other systems, such as W(Ti), where the alloying had a significant influence on the stress state of the film. Understanding this behavior could not only help mitigate the stresses inherent to thin film synthesis, but also guide the future design of thermally stable bulk nanocrystalline alloys.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. David Stepp
Division Chief
Program Manager, Mechanical Behavior of Materials
Program Manager (Acting), Synthesis and Processing of Materials

Dr. John Prater
Program Manager, Materials Design

Dr. Chakrapani (Pani) Varanasi
Program Manager, Physical Properties of Materials

Dr. Julia Barzyk
Program Manager, Earth Materials and Processes

B. Directorate Scientists

Dr. David M. Stepp
Director (Acting), Engineering Sciences Directorate

Dr. April Brown (IPA)
Research Scientist

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. LaToya Guidry
Administrative Specialist

CHAPTER 8: MATHEMATICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2016* is to provide information on the programs and basic research supported by ARO in fiscal year 2016 (FY16), and ARO's mission to create basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Mathematical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY16.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mathematical Sciences Division supports research to develop a foundational framework for the understanding and modeling of complex nonlinear systems, for stochastic networks and systems, for mechanistic models of adaptive biological systems and networks, and for a variety of partial differential equation (PDE) based phenomena in various media. These research areas focus on discovering nonlinear structures and metrics for modeling and studying complex systems, creating theory for the control of stochastic systems, spatial-temporal statistical inference, data classification and regression analysis, predicting and controlling biology through new hierarchical and adaptive models, enabling new capabilities through new bio-inspired techniques, creating new high-fidelity computational principles for sharp-interface flows, coefficient inverse problems, reduced-order methods, and computational linguistic models. This research will ensure the U.S. is on the research frontier in mathematical sciences, and will enable new advances in disciplines that depend on mathematics.

2. Potential Applications. Research managed by the Mathematical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. Long term basic research discoveries regarding the modeling of complex systems may enable full (*i.e.*, not only physical) situational awareness through modeling of urban terrain and small-group social phenomena. Outcomes of basic research in probability and statistics may provide enhanced levels of information assurance, improved awareness of and defense against terrorist threats, next generation communication networks, and improved weapon design, testing, and evaluation. New discoveries in biomathematics may lead to protection against future biological and chemical warfare agents, improve wound-healing, lead to self-healing communication networks, enhance cognitive capabilities for the Soldier, and contain or prevent infectious disease. Advances from basic research in the area of numerical analysis may enable faster/better analysis, design, prediction, real-time decision making, and failure autopsy.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives and to maximize the impact of potential discoveries for the Army and the nation, the Mathematical Sciences Division frequently coordinates, leverages, and transitions research within its Program Areas with ARL Campaign scientists and engineers, such as in Assessment and Analysis (e.g., novel mathematically rigorous statistical reliability and survivability methods), Computational Sciences (e.g., stochastic quantum differential equations for quantum computing), Human Sciences (e.g., structured methods for machine translation of low resource languages), Information Sciences (e.g., mathematical formulation of the dynamics of topologically-changing communication systems which serve as basis of system control methods), Materials Research (e.g., mathematics of incommensurability for multiscale modeling of 2-D materials), Sciences for Maneuver (e.g., isogeometric analysis for turbine design), and Sciences for Lethality and Protection (e.g., design of experimental techniques for meager data sets). It also coordinates and leverages research with other DoD agencies such as the Office of Naval Research (ONR) and the Air Force Office of Scientific Research (AFOSR).   In addition, the Division

frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the Network Sciences Division pursue common interests in cognitive modeling, bio-network modeling and design, and new concepts in computational optimization. The Mathematical Sciences Division also coordinates its research portfolio with the Computing Sciences Division to promote investigations of new architectures and algorithms for the future of heterogeneous computing and to pursue related interests in image recognition and information fusion. Research also complements initiatives in the Life Sciences Division to model and understand the relationship between microbial growth conditions and composition, leading to advances in microbial forensics. The creation of new computational methods and models to better understand molecular structures and chemical reactions are an area of collaboration between the Chemical Sciences and Mathematical Sciences Divisions. The Mathematical Sciences Division also coordinates its research portfolio with the Physics Division to pursue fundamental research in the stochastic PDEs of quantum control. The Division interfaces with Program Areas in the Mechanical Sciences Division to explore the mechanics of fluids in flight and to better understand combustion. These interactions promote synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

The Mathematical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY16, the Division managed research within these four Program Areas: (i) Modeling of Complex Systems, (ii) Probability and Statistics, (iii) Biomathematics, and (iv) Computational Mathematics. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Modeling of Complex Systems. The goal of this Program Area is to develop quantitative models of complex, human-based or hybrid physics and human-based phenomena of interest to the Army by identifying unknown basic analytical principles and by using human goal-based metrics. Complete and consistent mathematical analytical frameworks for the modeling effort are the preferred context for the research, but research that does not take place in such frameworks is considered if the phenomena are so complex that such frameworks are not feasible. The identification of accurate metrics is part of the mathematical framework and is of great interest, as traditional metrics often do not measure the characteristics in which observers in general, and the Army in particular, are interested. For many complex phenomena, new metrics need to be developed at the same time as new models. This Program Area is divided into two research thrusts: (i) Geometric and Topological Modeling and (ii) Small-group Social and Sociolinguistic Modeling. In FY13, the Modeling of Complex Systems Program included legacy efforts in information fusion. New efforts in information fusion will be part of the Information Processing and Fusion Program in the ARO Computing Sciences Division.

This Program Area develops mathematical analysis for fully 3D (rather than 2.5D) geometric and topological modeling of large urban regions up to 100 km x 100 km, which is important for situational awareness, mission planning and training. It develops the quantitative, analytical models of small social groups and of sociolinguistic phenomena which are required for operations, training, simulation (computer generated forces) and mission planning.

2. Probability and Statistics. The goal of this Program Area is to create innovative theory and techniques in stochastic/statistical analysis and control. Basic research in probability and statistics will provide the scientific foundation for revolutionary capabilities in counter-terrorism, weapon systems development, and network-centric warfare. This Program Area is divided into two Thrust areas: (i) Stochastic Analysis and Control, and (ii) Statistical Analysis and Methods.

The goal of the Stochastic Analysis and Control Thrust is to create the theoretical foundation for modeling, analysis, and control of stochastic networks, stochastic infinite dimensional systems, and open quantum systems. Many Army research and development programs are directed toward modeling, analysis, and control of stochastic dynamical systems. Such problems generate a need for research in classical and quantum stochastic processes, random fields, and/or classical and quantum stochastic differential equations in finite or infinite

dimensions. These systems often have non-Markovian behavior with memory for which the existing stochastic analytic and control techniques are not applicable. The research topics in this Thrust include, but are not limited to, the following: (i) analysis and control of stochastic delay and partial differential equations; (ii) complex and multi-scale networks; (iii) spatial-temporal event pattern analysis; (iv) quantum stochastics and quantum control; (v) stochastic pursuit-evasion differential games with multi-players; and (vi) other areas that require stochastic analytical tools.

The objective of the Statistical Analysis and Methods Thrust is to create innovative statistical theory and methods for network data analysis, spatial-temporal statistical inference, system reliability, and classification and regression analysis. The research in this Thrust supports the Army's need for real-time decision making under uncertainty and for the design, testing and evaluation of systems in development. The following research topics are of interest to the Army and are important for providing solutions to Army problems: (i) Analysis of very large or very small data sets, (ii) reliability and survivability, (iii) data, text, and image mining, (iv) statistical learning, (v) data streams, and (vi) Bayesian and non-parametric statistics, (vii) statistics of information geometry, and (viii) multivariate heavy tailed statistics.

Potential long-term applications for research carried out within this Program Area include optimized design and operation of robust and scalable next-generation mobile communication networks for future network-centric operations made possible through advances in stochastic network theory and techniques. Also, advances in stochastic fluid turbulence and stochastic control of aerodynamics can improve the maneuvering of helicopters in adverse conditions and enable optimal design of supersonic projectiles. In addition, new results in density estimation of social interactions/networks will help detect adversarial behaviors and advances in spatial-temporal event pattern recognition and will enable mathematical modeling and analysis of human hidden intention and will provide innovative approaches for counter-terrorism and information assurance. Finally, new discoveries in signature theory will significantly improve reliability of Army/DoD systems and experimental design theory, and will lead to accurate prediction and fast computation for complex weapons.

3. Biomathematics. The goal of this Program Area is to identify and mathematize the fundamental principles of biological structure, function, and development across biological systems and scales. The studies in this program may enable revolutionary advances in Soldier health, performance, and materiel, either directly or through bio-inspired methods. This Program Area is divided into three main research Thrusts: (i) Multiscale Modeling/Inverse Problems, (ii) Fundamental Laws of Biology, and (iii) Modeling Intermediate Timescales. Within these thrusts, basic, high-risk, high pay-off research efforts are identified and supported to achieve the program's long-term goals. Research in the Multiscale Modeling/Inverse Problems Thrust involves creating mechanistic mathematical models of biological systems at different temporal and/or spatial scales and synchronizing their connections from one level of organization to another, with the goal of achieving a deeper understanding of biological systems and eventually connecting top-down and bottom-up approaches. Research in the Fundamental Laws of Biology Thrust is high-risk research in biomathematics at its most fundamental level, seeking to find and formulate in a mathematical way the basic, general principles underlying the field of biology, a feat that has been performed for other fields, such as physics, but is in its infancy with respect to biology. Efforts in the Modeling at Intermediate Timescales Thrust attempt to develop new methods of modeling of biological systems, as well as their control, at intermediate timescales.

While these research efforts focus on high-risk, high pay-off concepts, potential long-term applications for the Army include new and better treatments for biowarfare agent exposure, improved military policies on troop movements in the presence of infectious disease, optimized movements of groups of unmanned autonomous vehicles and communications systems, and improved understanding of cognition, pattern recognition, and artificial intelligence efforts. Research in this Program Area could also lead to improved medical diagnoses, treatments for disease, limb regeneration, microbial forensics, detection of terrorist cells, and self-healing networks. Finally, efforts within this program may result in a revolutionized understanding of biology in general, which will at the very least allow future modeling efforts to be much more efficient and also undoubtedly have far-reaching effects for the Army in ways yet to be imagined.

4. Computational Mathematics. The goal of this Program Area is to develop a new mathematical understanding to ultimately enable faster and higher fidelity computational methods, and new methods that will enable modeling of future problems. The research conducted within this program will enable the algorithmic analysis of current and future classes of problems by identifying previously unknown basic computational

principles, structures, and metrics, giving the Army improved capabilities and capabilities not yet imagined in areas such as high fidelity modeling, real-time decision and control, communications, and intelligence. This Program Area is divided into three research Thrusts: (i) Multiscale Methods, (ii) PDE-Based Methods, and (iii) Computational Linguistics. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. The goal of research in the Multiscale Methods Thrust is to achieve higher fidelity and more efficient modeling of multiscale phenomena in a variety of media, and to create general methods that make multiscale modeling accessible to general users. Efforts in the PDE-Based Methods Thrust focus on developing the mathematics required for higher fidelity and more efficient modeling of sharp-interface phenomena in a variety of media, to discover new methods for coefficient inverse problems that converge globally, and to create reduced order methods that will achieve sufficiently-accurate yet much more efficient PDE solutions. Efforts in the Computational Linguistics Thrust focus on creating a new understanding of natural language communication and translation through new concepts in structured modeling.

While these research efforts focus on high-risk, high payoff concepts, potential long-term applications for the Army include force protection concrete and improved armor, more stable but efficient designer munitions, high density, rapid electronics at low power, and nondestructive testing of materials. Program efforts could also lead to more capable and robust aerial delivery systems, more efficient rotor designs, systems to locate explosive materials, more efficient combustion designs, and real-time models for decision-making. Finally, efforts within this program may lead to natural language interactions between bots and humans in cooperative teams, new capabilities for on-the-ground translation between deployed U.S. forces and locals, especially in low-resource language regions, new and improved capabilities for automated translation, automatic summarization, and textual analysis within the strategic intelligence communities.

C. Research Investment

The total funds managed by the ARO Mathematical Sciences Division for FY16 were $24.1 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY16 ARO Core (BH57) program funding allotment for this Division was $6.1 million and $1.9 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $8.0 million to projects managed by the Division. The Division also managed $4.8 million of Defense Advanced Research Projects Agency (DARPA) programs and $0.6 million was provided by other Army Laboratories. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.0 million for contracts. In addition, $2.7 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $1.0 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY16 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY16 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY16, the Division awarded 11 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Radu Balan, University of Maryland - College Park; *Nonlinear and Probabilistic Analysis with Frames*
- Professor Maria Chudnovsky, Princeton University; *Coloring Perfect Graphs*
- Professor Evan Drumwright, George Washington University; *Adaptive Integration of Nonsmooth Dynamical Systems*
- Professor Andrew Glen, The Colorado College; *Explorations of Hybrid Symbolic-Probabilistic Mathematics*
- Professor Carl Kelley, North Carolina State University; *Inverse Bathymetry Problems*
- Professor Dima Krioukov, Northeastern University; *Structural Properties of Random Graphs and Simplicial Complexes*
- Professor Hideo Mabuchi, Stanford University; *Dimension Reduction for Open Quantum Systems*
- Professor Boris Rozovsky, Brown University; *Deterministic Approach to Solving Stochastic Partial Differential Equations (PDEs)*
- Professor Guillermo Sapiro, Duke University; *Multimodal Subspace Learning and Modeling of Complex Systems*
- Professor Semyon Tsynkov, North Carolina State University; *Numerical Simulation of Time-Dependent Waves with High Order Accuracy and Interfaces of General Shape*
- Professor Evan Variano, University of California - Berkeley; *Turbulence, Symmetry, and the Role of Organism Shape in Perception*

2. Short Term Innovative Research (STIR) Program. In FY16, the Division awarded four new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Tomas Arias, Cornell University; *Density Functional Theory as a New Mathematical Framework for Predicting Population Flows*

- Professor Shingchang Kou, Harvard University; *Multi-level Hidden Markov Model for Co-translational Protein Targeting*

- Professor Daisuke Takagi, University of Hawaii - Honolulu; *Modeling the Collective Behavior of Unsteadily Swimming Zooplankton*

- Professor Suriyanarayanan Vaikuntanathan, University of Chicago; *Principles of Organization in Biological Systems*

3. Young Investigator Program (YIP). In FY16, the Division awarded one new YIP project to drive fundamental research in areas relevant to the current and future Army. The following PI and corresponding organization was a recipient of the new-start YIP award.

- Professor Padmini Rangamani, University of California - San Diego; *Multiscale Models of Cell Motility*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY16 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Conference on Applied Statistics in Defense*; Fairfax, VA; 21-23 October 2015

- *Mathematics and the Quest for Fundamental Principles of Biology*; Salt Lake City, UT; 14-15 December 2015

- *XXXV Dynamics Days*; Durham, NC; 7-10 January 2016

- *Joint 2016 MBI-NIMBioS CAMBAM Summer Graduate Workshop on Mathematical Modelling of Infectious Diseases*; Knoxville, TN; 13-22 June 2016

- *Mathematical and Computational Aspects Related to Soil Modeling and Simulation*; Chicago, IL; 1-2 August 2016

- *Workshop on Quantum Stochastic Differential Equations for the Quantum Simulation of Physical Systems*; Adelphi, MD; 22 August 2016

- *Teaching the Theory in Density Functional Theory*; Los Angeles, CA; 22-26 August 2016

5. Special Programs. In FY16, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded four new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Mathematical Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Measuring, Understanding, and Responding to Covert Social Networks: Passive and Active Tomography. This MURI began in FY10 and was awarded to a team led by Professor Joseph Blitzstein at Harvard University. The goal of this MURI is to develop quantitative procedures to identify, characterize and display, on the basis of externally observed data generated from passive and/or active procedures, covert social networks of asymmetric adversaries, that is, terrorist/insurgent networks.

In its first three years, the MURI team developed a framework for quantifying the fundamental limits of detectability for embedded insurgent sub-networks. This first rigorous "signal detection theory" for networks enables the computation of these performance limits within a coherent mathematical framework and the development of algorithms that approach them. This theory enables one to make trade-offs between algorithmic performance and computational requirements.

The team has encoded society+network connections (e.g., adjacency matrix with elements $\neq 0$ if tie exists) to fit a benign-background model to the encoded society+network model, fit a notional signal-plus-clutter model to

partitions of the society+network model to make network signal stand out from clutter, and has begun work on statistically testing for signal presence and for use structure to localize the network in society. This is the first known rigorous signal detection theory for networks in a decision-theoretic framework.

In the fourth year of investigation, the MURI team has defined the various threads within community detection models. Within each thread, the team has developed mathematical models that are based on sociological processes which tackle subgroup detection with respect to different sociological process (language, geolocation, densities of interaction, etc.). Each of these efforts demonstrates mathematical richness, with some apparent possibility to move closer to establishing error bounds on predictions. The emphasis has remained on detection rather than general theory, has based simulation structure on real terrorist networks with quality control evaluations, and continues to emphasize the tri-thrust framework of linking social theory to mathematics, simulation and testing, and social data.

2. Structured Modeling for Low Resource Translation. This MURI began in FY10 and was awarded to a team led by Professor Jaime Carbonell at Carnegie Mellon University. The goal of this MURI is to investigate new concepts for language translation that use structured modeling approaches rather than solely statistical methods.

Whereas statistical approaches for machine translation (MT) and text analysis (TA) successfully harvest the low-hanging fruit for large data-rich languages, these approaches prove insufficient for quality MT among typologically-diverse languages and, worse-yet, are inapplicable for very low-resource languages. This research is venturing much further than just introducing syntactical structures into statistical machine translation and will turn the process on its head (*i.e.*, start with a true linguistic core and add lexical coverage and corpus-based extensions as data availability permits). This linguistic core will comprise an enriched feature representation (morphology, syntax, functional semantics), a suite of core linguistic rules that operate on these features via powerful operators (tree-to-tree transduction, adjunction, unification, etc.), and prototype MT and TA engines to evaluate their accuracy and phenomenological coverage. Contrastive linguistic analysis will identify the major translation divergences among typologically diverse languages, feeding into the MT linguistic core. Once the core is built, coverage will be broadened through additional linguist-generated rules and via Bayesian constraint learning from additional corpora and annotations as available; learning with strong linguistic priors, respecting the linguistic core, is expected to require much less data than unconstrained corpus-based statistical learning. The initial efforts are focusing primarily on African languages, such as Chichewa and Kinyarwanda (Bantu family), Tumak (an Afro-Asiatic Chadic language), Dholuo (a Nilo-Saharan language), and for even greater typological diversity, Uspanteko (a Mayan language). In addition to designing, creating, and delivering the linguistic cores for the selected languages, this research focuses on delivering a suite of methods and algorithms (*e.g.*, tree-to-tree feature-rich transducers, proactive elicitors) and their prototype software realizations.

The new powerful linguistic capabilities potentially generated by this research will enable the Army to perform rapid and principled construction of MT and TA systems for very diverse low-density/low-resource languages. This has the potential to provide the Army with new tactical capabilities for on-the-ground translation between deployed US forces and locals, especially in low density language regions. It also has the potential for new and improved capabilities for automated translation, automatic summarization, and textual analysis within the strategic intelligence communities.

3. Optimal Control of Quantum Open Systems. This MURI began in FY11 and was awarded to a team led by Professor Daniel Lidar of the University of Southern California. The goal of this MURI is to show a high degree of fundamental commonality between quantum control procedures spanning all application domains.

This research is pursuing the development of a new mathematical theory unifying quantum probability and quantum physics, and this research is developing new ideas in quantum control that are presently in their infancy. Of particular importance is perhaps the most pressing quantum control frontier: real-time coherent feedback control of non-Markovian open systems. To address this goal, the team is studying unifying features of controlled quantum phenomena. The means for achieving quantum control is generally categorized as either open-loop control, adaptive open-loop control, real-time feedback control, or coherent real-time feedback control. Despite the operational distinctions between these control categories, the researchers aim to show that there is a strong relationship between all of these approaches to control, using algebraic and topological techniques. This linkage is expected to be significant for seamlessly melding these tools together in the

laboratory to draw out the best features of each method for meeting new control challenges and overcoming inevitable laboratory constraints, such as the context of proposed meso-scale laser and atomic Rb experiments.

4. Multivariate Heavy Tail Phenomena: Modeling and Diagnostics. This MURI began in FY12 and was awarded to a team led by Professor Sidney Resnick of Cornell University. The project aims to develop reliable diagnostic, inferential, and model validation tools for heavy tailed multivariate data; to generate new classes of multivariate heavy tailed models that highlight the implications of dependence and tail weight; and to apply these statistical and mathematical developments to the key application areas of network design and control, social network analysis, signal processing, network security, anomaly detection, and risk analysis.

More specifically, the researchers are investigating and developing statistical, mathematical, and software tools that will provide (i) flexible and practical representations of multidimensional heavy tail distributions that permit reliable statistical analysis and inference, allow model discovery, selection and confirmation, quantify dependence, and overcome the curse of dimensionality, (ii) heavy tailed mathematical models that can be calibrated which clearly exhibit the influence of dependence and tail weight and which are appropriate to the applied context, and (iii) exploitation of the new tools of multivariate heavy tail analysis to enable the study of social networks, packet switched networks, network design and control, and robust signal processing.

5.   Associating Growth Conditions with Cellular Composition in Gram-negative Bacteria. This MURI began in FY12 and was awarded to a team led by Professor Claus Wilke of the University of Texas - Austin. The goal of this research is to develop methods to identify statistical association in multiple-input-multiple-output (MIMO) data using microbial growth and composition data.

To trace a microbe-causing disease to its source or to predict a microbe's phenotype in a given environment, it is necessary to be able to associate the conditions under which bacteria have grown with the resulting composition of the bacterial cell. However, the input and output data complexity – multiple, heterogeneous, and correlated measurements – poses an interpretational challenge, and novel methods for analyzing, integrating, and interpreting these complex MIMO data are sorely needed. The research team is thus comprised of experts in statistics, computational biology, computer science, microbiology, and biochemistry, with the goal of producing the following outcomes: (i) development of novel linear and nonlinear mathematical methods to associate bacterial cellular composition with growth conditions, (ii) identification of the types and ranges of growth conditions that lead to distinguishable cellular composition, (iii) identification of key compositional markers that are diagnostic of specific bacterial growth conditions, and (iv) assessment of model uncertainty, robustness, and computational cost. The MURI will develop capabilities in several novel areas of data analysis and statistics such as the analysis of MIMO data, the integration of side information into regression models, and inverse optimization approaches. In addition, the types of approaches developed in this project will advance DoD capabilities in bacterial forensics and enable natural outbreaks to be distinguished from intentional attacks.

6.   *Understanding the Skin Microbiome.* This MURI began in FY14 and was awarded to a team led by Professor David Karig of the Applied Physics Lab at the Johns Hopkins University. The goal of this research is to develop a fundamental understanding of the forces shaping skin microbial communities across a range of spatial scales and to show how this understanding can be used to identify disease risk, predict disease outcomes and develop tools for disease prevention.

Human skin harbors diverse bacterial communities that vary considerably in structure between individuals and within individuals over time. The extent of this variability and its implications are not fully understood, nor is it known whether it is possible to predict what types of bacteria one is likely to find on the skin of a given individual. As a result, there are no effective tools to predict individuals more likely to acquire skin bacterial infections, then determine the efficacy of forensic analyses based on skin bacterial communities, nor to design novel strategies to limit the effective colonization of skin by pathogens. This project brings a variety of disciplines to bear on the problem: spatially explicit sampling, metagenomics, and bioinformatics will be used to characterize skin microbial communities at intermediate and large spatial scales. Molecular biology, analytical chemistry and synthetic biology will be used to probe smaller-scale processes that ultimately lead to larger-scale patterns. Ecological modeling will be used to integrate small-scale processes with large-scale patterns in order to arrive at a quantitative and predictive framework for interpreting the human skin microbiome.   A series of models concentrating on four grand challenges will be built, tested and refined: (i) predicting microbiome composition based on environmental conditions, host state and microbe exposure patterns, (ii) identifying microbiome composition through volatile sensing, (iii) identifying disease risk through analysis of current state

and anticipation of state changes, e.g., due to upcoming activities or events, and (iv) novel approaches for mitigating skin disease (e.g., optimal design of avoidance behavior, robustly engineered skin microbiomes). The results of this work will enable the manipulation of the skin microbiome in order to facilitate identification of allies, discourage bites of flying insects, predict skin disease, and as-yet-unimagined applications.

7. Strongly Linked Multiscale Models for Predicting Novel Functional Materials. This MURI began in FY14 and was awarded to a team led by Professor Mitch Luskin at University of Minnesota. The goal of this research is to investigate mathematical methods for strongly linking scales within the context of discovering novel functional materials.

Current research in multiscale modeling has moved little beyond weak dependence between continuum and atomistic models. In commonly-used weakly linked multiscale models, a macroscale exerts at most a homogeneous influence on a greatly separated finer scale and lacks constitutive properties, which are supplied by reaching down to the smaller scale to compute, average, and report back. Such weak multiscaling dilutes or eliminates nonlinearities and the resulting models misrepresent the observed macroscale behavior. Variabilities in microfunctional parameters not only generate uncertainty within a scale, but also propagate uncertainties between scales, both up and down, resulting in a potentially significant spread in macroscopic properties. Removing degrees of freedom from a dense system during upscaling may result in loss of information that can only be accounted for by introducing suitable random and dissipative forces that render the final mathematical formulation stochastic. This project seeks to develop a mathematical foundation for a computational framework of several strongly linked scale models for functional materials, with attendant uncertainty quantification. This will be developed within the framework of designing and discovering novel perovskite materials, mismatched alloy semiconductor materials, and 2D nanomaterials with unprecedented functional properties.

8. Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications. This MURI began in FY16 and was awarded to a team led by Professor George Karniadakis at Brown University. The goal of this research is to develop a new rigorous theoretical and computational framework enabling end-to-end fractional modeling of physical problems governed by conservation laws in large-scale simulations.

Despite significant progress over the last 50 years in simulating complex multiphysics problems using classical (integer order) partial differential equations (PDEs), many physical problems remain that cannot be adequately modeled using this approach. Examples include anomalous transport, non-Markovian behavior, and long-range interactions. Even well-known phenomena such as self-similarity, singular behavior, and decorrelation effects are not easily represented within the confines of standard calculus. This project seeks to break this deadlock by developing a new class of mathematical and computational tools based on fractional calculus, advancing the field in specific areas of computational mechanics. The fractional order may be a function of space-time or even a distribution, opening up great opportunities for modeling and simulation of multiscale and multiphysics phenomena based on a unified representation. Hence, data-driven fractional differential operators will be constructed that fit data from a particular experiment, including the effect of uncertainties, in which the fractional PDEs (FPDEs) are determined directly from the data.

The work is addressing the fundamental issues associated with the construction of fractional operators for conservation laws and related applications. An integrated framework is being pursued that proceeds from the initial data-driven problem to ultimate engineering applications. This general methodology will allow the development of new fractional physical models, testing of existing models, and assessment of numerical methods in terms of accuracy and efficiency. The integrated framework is based on a dynamic integration of five areas: (i) mathematical analysis of FPDEs; (ii) numerical approximation of FPDEs; (iii) development of fast solvers; (iv) fractional order estimation and validation, from data; and (v), prototype application problems.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program has a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY16, the Division managed one new-start Phase II SBIR contract, in addition to active projects continuing from prior years. This new-start contract aims to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY16 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES. In FY16, the Division managed two new-start Phase II STTR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of STTR topics published in FY16 and a list of prior-year STTR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY16, the Division managed one new ARO (Core) HBCU/MI project and four new REP awards, in addition to active projects continuing from prior years. Refer to CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

There were no new starts in FY16.

G. Defense University Research Instrumentation Program (DURIP)

As described in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY16, the Division managed three new DURIP projects, totaling $0.8 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Biochronicity Program

The DARPA Biochronicity Program builds on studies from the DARPA Fundamental Laws of Biology (FunBio) Program. ARO co-developed the Biochronicity Program, and currently co-manages the program as a core component of the ARO Biomathematics Program's emphasis on identifying the fundamental mathematical principles of biological structure, function and development applied across different biological systems and scales. The Biochronicity program in particular seeks to achieve a fundamental understanding of the role of time in biological functions in order to be able to manage the effects of time on human physiology. For example, biological clocks are involved in regulating virtually every function of the human body, yet exactly how time contributes to cell-cycle progress, growth, metabolism, aging, and cell death is unclear. In order to understand the coordination of timing on multiple scales in the human body, the Biochronicity program uses an interdisciplinary approach, involving empirical data sets, mathematical modeling, bioinformatics techniques, statistics, and data-mining, to identify common spatio-temporal instructions, or "clock signatures," regulating various physiological systems. Understanding how time regulates human biological processes should allow one to manipulate these processes so that one can for example improve trauma care on the battlefield by increasing the time available for medical treatment and surgery, as well as decrease the deleterious effects of age-related diseases and other infirmities. Along with the clear DoD relevance of the program, efforts in the Biochronicity program are leveraged by the Division's Biomathematics Program Area, Fundamental Laws of Biology Thrust.

I. DARPA Enabling Quantitative Uncertainty in Physical Systems (EQUiPS) Program

The DARPA EQUiPS Program builds on previous work in uncertainty quantification. Complex physical systems, devices, and processes important to the DoD are often poorly understood due to uncertainty in models, parameters, operating environments, and measurements. The goal of this program is to provide a rigorous

mathematical framework and advanced tools for propagating and managing uncertainty in the modeling and design of complex physical and engineering systems. ARO co-manages awards within this Program. Of particular interest are systems with multi-scale coupled physics and uncertain parameters in extremely high-dimensional spaces. Novel mathematical research is being developed for dealing with the underlying high dimensionality of the space of uncertain parameters, strong multi-physics coupling, and uncertainty in the models themselves. In addition, the lack of fundamental mathematical theory for decision making and design under uncertainty for these large-scale dynamic systems is being addressed though new methods for forward and inverse modeling to scale to high-dimensional multi-scale/multi-physics systems, a quantitative understanding of uncertainties and inadequacies in the physical models themselves, and a completely new paradigm for stochastic design and decision making for complex systems. This work helps further the work done in the Division's Computational Mathematics Program Area, Mathematics of Multiscale Modeling Thrust.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Mathematical Sciences Division.

A. Structured and Collaborative Geometric Signal Models for Big Data Analysis
Professor Guillermo Sapiro, Duke University, Single Investigator Award

The objective of this research is to identify and develop the mathematical principles best-suited for models of ill-posed reconstruction, classification, and identification problems in data and signal analysis. It has been carried out by combining aspects of classical signal modeling theory with theories from sparse and subspace modeling, Gaussian mixture models (GMMs), and low rank transformation methods. The effort focused primarily on audio and video signals, as well as photographic data and object/facial recognition problems, both in visible, infrared (IR), and near-infrared (NIR) light. The aforementioned "ill-posed" characteristic of the data analysis problems of interest refers to the data having adverse properties that make processing using classical methods much more difficult, if not altogether impossible, including data being corrupted and/or having missing or heavily obscured features. In the context of facial recognition, for instance, a captured video image of a person's face might be affected by lighting conditions which obscure part of the face either through glare or shadow, the angle of the face relative to the camera (i.e. only a partial shot may be available to compare to images in a database), or even variations in the facial expression that alter its appearance. Success of the research has been measured in terms of processing speed and accuracy, as well as robustness, particularly as compared with more traditional methods.

In FY16, the problem has been approached from a machine learning perspective, seeking to not only train an algorithm to overcome undersampled, missing, or tainted data to process and analyze a signal, but to do so by learning the signal model in situ, based directly on the compressive measurements of the signal and without resorting to other signals for training. This is, in some sense, a realistic necessity when using GMMs, since an accurate GMM training signal model that matches the statistics of the signals being sensed is not generally available a priori. However, it also means that the algorithm can train and operate simultaneously, which is a clear advantage in both operating time and cost, as well as in training data requirements.

This framework was achieved by utilizing an innovative, compressed sensing approach in concert with a combination of classical and new tools from sparse modeling in information theory. Solving the problem of compressive sensing via learning a GMM from direct measurements instead of training data was a significant breakthrough in the latter research stages of this effort. This was achieved by treating the signals being sensed as random variables and integrating them out in the likelihood. In turn, a maximum marginal likelihood estimator (MMLE) was derived that maximizes the likelihood of the GMM of the underlying signals given only their linear compressive measurements. Extending the MMLE to a GMM with dominantly low-rank covariance matrices yielded computational speedup.

The signal modeling advances were achieved largely by using subspace methods. More specifically, the algorithm was trained to learn a global linear transformation on a collection of subspaces, doing so in such a manner as to reduce the variations within, while increasing the separation between, subspaces. When combined with an also newly developed framework for carrying out binary hashing on random forests, along with the previously described compressive sensing tools, the result was a much faster and more computationally efficient signal processing framework than has been previously known. In the context of face and object recognition, in particular, the result was an ultra-fast, state-of-the-art recognition tool that is not only significantly faster and requires orders of magnitude less training data and time than competing algorithms, but is quantifiably more accurate and notably more robust, being able to correctly identify objects and faces in multiple light spectra and with sparse data (see FIGURE 1).
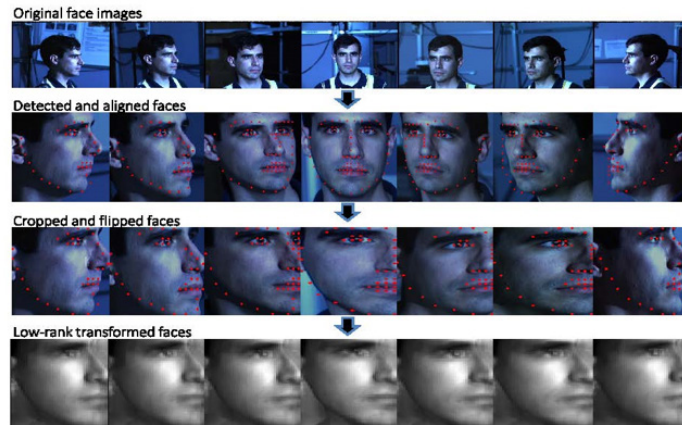
FIGURE 1

Fast Facial Recognition. The last row shows that under this framework, each original, captured image (first row) leads to detection of the correct subject from the database, regardless of orientation of the subject or distortion of the appearance.

It was anticipated that, in addition to gains in computational speed and efficiency, an increase in object and facial recognition accuracy of 10% could be achieved. The results of the project were, in many cases, even more pronounced than this, which should enable better performance in signal reconstruction, classification, and identification in adverse conditions. In the case of IR face/object recognition, this new tool produced a 16% improvement in recognition accuracy using Oxford's Visual Geometry Group-Face dataset (VGG-Face, which is generally thought of as the best face model available in the literature), and a 10% improvement in accuracy using the CASIA-NIR-VIS, the largest near infrared-vs.-visual light face recognition benchmark. Furthermore, the particular subspace learning framework developed in the signal modeling phase was shown, using fundamental theory, to be the only one that can achieve the desired data behavior. With regard to computational cost, computation time, and learning/training time, this framework resulted in an improvement in the context of facial recognition by 5-to-6 orders of magnitude. Finally, by applying geometric transformation techniques to the learning algorithms, it was shown that the algorithms' robustness could be increased within these new frameworks, yielding improvements of 5-7% on the Mixed National Institute of Standards and Technology (MNIST) database and 2% on the Faces on the Wild database. The latter improvement is small but noteworthy, as that facial image database is known to be large and complex, making any small improvement in recognition accuracy significant.

B. Nonlinear Stochastic PDEs: Analysis and Approximations
Professor Boris Rozovsky, Brown University, Single Investigator Award

The objective of this research is to create a universal approach to enable real-time approximation with small sequential data sets drawn from physical systems that are modeled by a class of nonlocal and nonlinear stochastic partial differential equations. Many physical dynamics, such as the canonical example of a fluid flow over a circular cylinder, are modeled by stochastic partial differential equations. There are two essential random perturbations affecting a system, a stochastic force acting directly upon the dynamic, or environmental factors that make the initial or boundary condition random.

In FY16, given the wealth of knowledge about fluid flows modeled by the Navier-Stokes equation, the PI focused on the exploration of creating these new and novel computational methods on this dynamic. A few other well researched dynamics the PI investigated to support the development of these computational methods include Euler equations for fluid flow, Burgers equations for shocked flow, and the stochastic Ginzburg-Landau equations for modeling superconductivity. From the initial investigations, the PI established two general methods of solution and computation to further develop: (i) the rigorous approximation of this class of stochastic partial differential equations; and (ii) the development of related fast computational algorithms.

The theoretical development of analytical techniques consisted of a novel leveraging of the well-known methods of generalized Malliavin calculus and generalized polynomial (Lévy) chaos. In particular, the PI had a unique

insight into the Wick-Malliavin representation of a stochastic partial differential equation. His insight led to the stochastic Fourier-like expansion of stochastic processes that separates the random terms and the deterministic terms. In this expansion, the closed form solutions of the random terms are known and the closed form solutions of the deterministic terms, which the PI defined as propagators, have to be inferred. For the majority of random dynamics, the propagator terms are partial differential equations related to the stochastic partial differential equation. While creating this expansion, the PI was looking for an intuitive term was sought that would demonstrate that further exploring and rigorously developing this method would be applicable to other disciplines. This was found with the first propagator term, which is the partial differential equation describing the dynamic of the physical process without any stochastic perturbations.

The theoretical technique the PI created bypasses the complexities of approximating the solution of the stochastic process, and simplifies the computation to solving a finite number of deterministic partial differential equations. The stochastic Fourier like expansion of the stochastic partial differential equation splits the numerical solution of the dynamic in two sequential steps: first the offline computation of the statistical moments of the solution, which includes the mean and variance; then the online solution using real-time data to determine the numerical solutions of the real-time propagators. While the common method to compute the statistical moments of the solution is the computationally expensive and time intensive Monte Carlo method, this technique allows for the immediate and explicit computation of all of the statistical moments.

Although theoretical work is still needed for computing the exact error of the approximation, the PI demonstrated with multiple examples an improvement in accurately modeling the underlying random physical process (see FIGURE 2). Simplifying the computation to deriving the propagator terms has decreased the computational complexity involved in finding a solution of the underlying random physical dynamic. As a consequence of these two methods, there is a significant decrease in the required number of sequential data points for approximating stochastic partial differential equations.
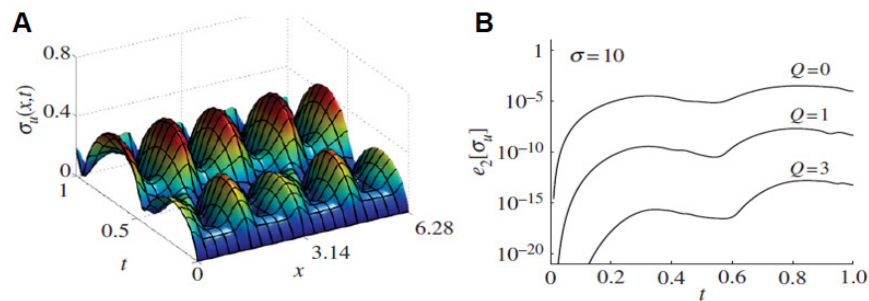

FIGURE 2

Burgers equation with additive random forcing perturbed by four random variables and variance $\sigma = 10$. (**A**) Standard deviation of the benchmark stochastic solution and (**B**) Convergence of the Wick–Malliavin approximation, where Q indicates the terms from the infinite sum included in the approximate stochastic process.

C. Fluid-Structure Interaction Simulation of Gas Turbine Engines Using Isogeometric Analysis
Professor Yuri Bazilevs, University of California at San Diego, Single Investigator Award

The objective of this research is to leverage recent developments in geometric modeling, coupled mechanical simulation such as fluid-structure interaction (FSI), and the integration of geometric modeling and simulation via isogeometric analysis, in order to develop new computational techniques for complex interacting domains such as those found in gas turbine engines and other applications. To investigate computational performance in these types of complex domains, a finite element-based formulation for the 3D compressible Navier–Stokes equations is used, but with the addition of a small number of curvilinear elements that are efficiently generated through level set methods and incorporate matching moments through the first few moments.

In FY16, it was found that using primitive variables rather than conservation variables enables re-writing the resulting system in a quasi-linear form relating the vector of primitive variables, the advective and diffusive fluxes, and a source term. Novel stabilization techniques were investigated to both better stabilize the formulation and to model the turbulence. While Eulerian frames are common in Computational Fluid Dynamics (CFD) applications, Arbitrary Lagrangian-Eulerian methods were investigated and adopted for compressible

flow in order to describe the flow inside the turbine passages, which include the spinning rotor and stationary stator vanes. The computational domain is partitioned into rotor and stator subdomains and coupled through a sliding interface. It was found that weakly enforced no-slip conditions can be imposed on the blade surfaces in order to avoid excessive resolution of the turbulent boundary layers.

A specific test case involved improving a new base turbine design currently being studied by ARL Sciences for Maneuver Campaign scientists. Modified rotor blade pitching as designed/iterated/optimized by these methods resulted in a 5.6% improvement in turbine-stage efficiency, which is a tremendous improvement in a system that has been already optimized by current methods (see FIGURE 3). This transformative capability fills the gap where computational methods were missing to begin carrying out designs using new high fidelity CFD and FSI.
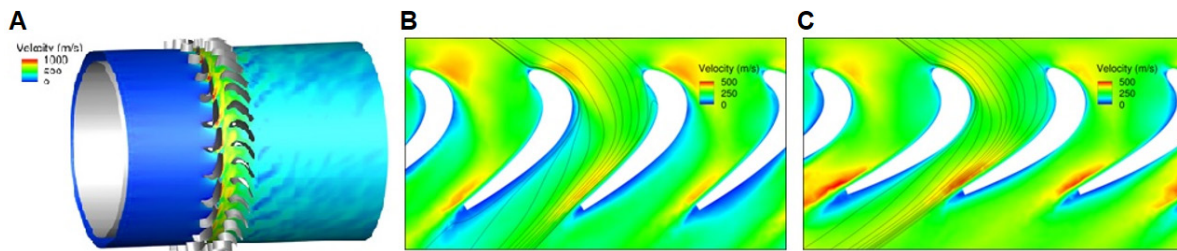

FIGURE 3

Single-passage simulation enables high mesh resolution in the turbine blade passages and better-understanding of the flow details. (A) Trivariate non-uniform rational basis splines for isogeometric analysis of fluid-structure interactions. (B) Phase lag boundary conditions enable simulating realistic rotating boundary conditions while restricting the simulation to just a single passage. (C) Modified rotor blade pitching improves efficiency of an already-optimized design by 5.6%.

The results from this research significantly advances the current state-of-the-art in isogeometric modeling and its applications to problems with multi-domains and complex interactions. This, in turn, will improve the ability to efficiently compute the solutions of large-scale systems that arise in the discretization of problems involving fluid-structure interaction. In the context of turbines, this work is expected to help lead to: (i) adaptive gas turbine blades for optimized engine performance; (ii) mitigated engine stall and flow separation in future turbine aircraft; and (iii) more efficient power generation.

D. Modeling Photoreceptive Ganglion Cells that Enable Subconscious Vision
   Professor Danny Forger, University of Michigan, Single Investigator Award

The objective of this research is to gain a better understanding of subconscious vision. For many years, scientists were puzzled at how many "blind" subjects could have subconscious physiological responses to light. In some subjects, light could cause pupil restriction or shift the internal daily (circadian) timekeeping system. About ten years ago, the source of this subconscious vision was discovered; a separate visual system exists that can function without rods or cones, and is solely based on retinal ganglion cells that become photoreceptive by expressing melanopsin (ipRGCs), a novel photo pigment which has different properties than Rhodopsin, which controls conscious vision. The aims of this research are to (i) model the intrinsic photoresponse of ipRGCs; (ii) model the electrophysiology of ipRGCs; (iii) model the inputs to ipRGCs from other parts of the retina; and (iv) determine what the ipRGC network can see. The PIs original work focused on the retina and then moved to the first part of the brain to receive signals from ipRGCs, the suprachiasmatic nucleus (SCN).

In FY16, as a result of achieving goal (i), ipRGCs were found to be able to be classified based on their responses into three main categories. Using mathematical modeling, the biophysical differences between these groups could be predicted. In developing the electrophysiology model of ipRGCs (goal ii), a mathematical question arose: given experimental data on the different ionic currents that affect the electrical activity of ipRGCs, can one determine the parameters of a model that is in the standard Hodgkin-Huxley form? This question was resolved largely in the affirmative using techniques from differential algebra. Given that ipRGCs are large cells in which spatial dynamics may play an important role, first recordings were generated from ipRGCs with their long dendrites removed so that the neuron would be small enough so that it could be directly compared to an ordinary differential equation model. Additionally, a partial differential equation model of ipRGCs was

developed to account for changes in the electrical activity in space and time, resulting in models of two important types of ipRGCs, M1 and M4 cells.

A working model of the retina also resulted based on the work involved in goal (iii). This model contains representations of all major parts of the retina, including rods, cones, bipolar cells, horizontal cells, amacrine cells, and retinal ganglion cells. The model contains about 1,000,000 cells and utilizes special GPU hardware for fast simulation which is being optimized and will be available for wide use.

The SCN is a very widely studied region of the brain and is the central daily clock that times daily events within the body. Its study is essential for the military, which must maintain alertness and readiness 24/7. Thousands of previous studies over the past 30 years have argued that the SCN integrates visual information from the entire visual field (rather than specific parts of the visual field), and uses information on overall light levels to time daily events. However, it was unclear why billions of action potentials in the SCN are needed for this relatively simple task. The PI, in collaboration with several experimental labs, showed that most individual SCN neurons are receptive for a small part of the visual field. Based on these experimental results, a new mathematical method was devised to determine the wiring of the SCN. The updated SCN model was also used to test whether the wiring of the SCN can enhance spatial visual tasks. Surprisingly, rather than smoothing and averaging spatial information, the SCN was found to enhance it, thus giving a new role to a key region of the brain.

One aspect of subconscious vision of particular importance to the DoD is gaze control, the ability of a mammal to move the center of the visual field onto a target. This research shows that the SCN greatly enhances this task (see FIGURE 4). Further study could provide key information on how nature locates targets.

Understanding subconscious vision will help improve understanding of vision in general, treatments to ameliorate the condition of the blind, and may allow better adjustment of the body's circadian clock so that our military can perform accurately 24/7. In fact, this research has resulted in several high profile papers, as well as an app, ENTRAIN, which has collected data on sleep patterns from thousands of individuals in over 100 countries. Using this data, differences were quantified in how much individuals sleep based on age, gender, and the country in which individuals live. For example, women schedule more sleep than men, and the effects of light due to subconscious vision's effects on the circadian clock had a much greater effect on the time at which one wakes up than the time at which one goes to sleep. This work received a tremendous amount of media attention including hundreds of media pieces in print, online, via radio and television.
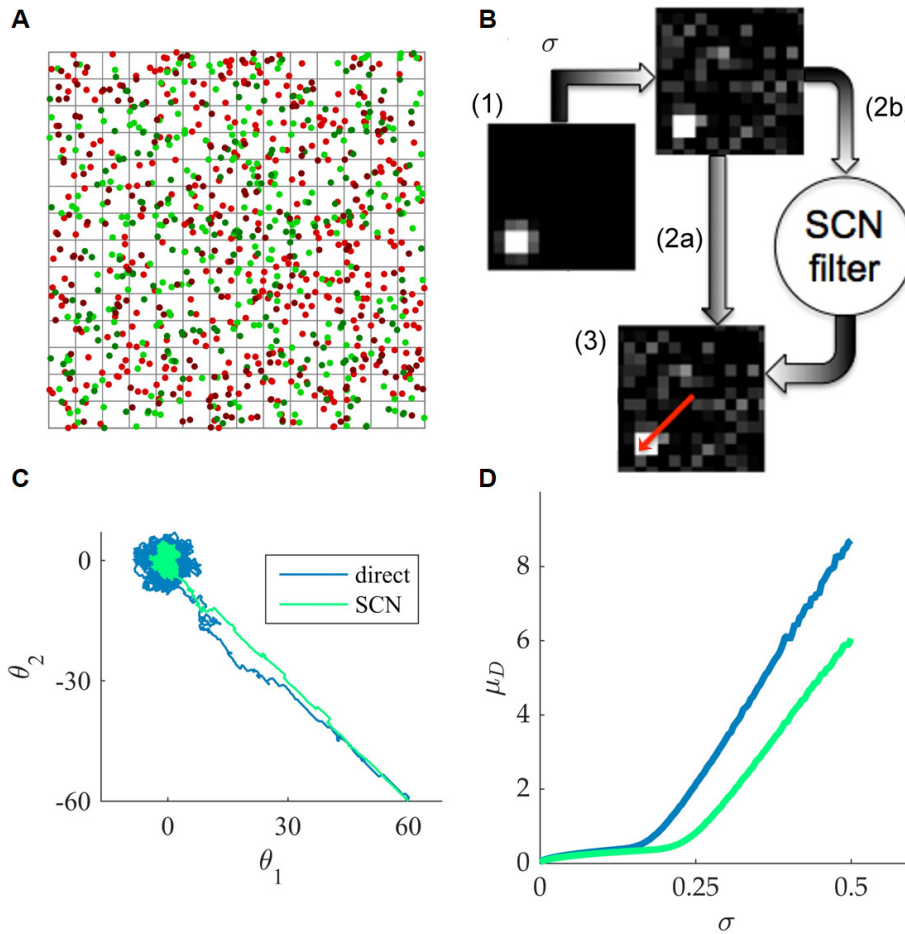
FIGURE 4

Tracking ability of a mammal to move the center of the visual field onto a target. Light receptive ganglion cells (ipRGCs) in the retina mediate subconscious vision. In mouse ~150 ipRGCs from each retina signal to the SCN. (**A**) These cells tile the retina, and each box shows the part of the visual scene that each cells responds to. The PI discovered that the SCN interpolates with the signals from the ipRGCs to give increased acuity of the visual scene. Plotted is the center of the receptive field of each SCN neuron in the model which gives many more pixels than the original ipRGC scene. (**B**) To test the role of the SCN in visual tasks it was determined the SCN could increase the ability of an animal to center a light source in the middle of its visual scene. The activation of ipRGCs by the light source is shown in (1), and noise typical of visual scenes is added (2). Study of a controller centering the light source in the center of the visual scene with inputs directly from the ipRGCs (2A) or the outputs of the SCN network (2B). (**C**) With the SCN the path towards the center of the visual scene, $\theta_1 = \theta_1 = 0$, is more direct than without the SCN input. (**D**) The jitter (μ_D) was also measured as a function of the noise level (σ). The SCN network reduced the amount of jitter in the visual scene.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Inferring Social and Psychological Meaning in Social Media (SURF)
Investigator: Tod Hagan, Securboration Inc., Small Business Innovation Research Award
Recipient: ARL Computational Sciences and Information Directorate (ARL-CISD)

The objective of this research is to develop analytical tools that use structured and non-structured social media information to identify significant topologies, motifs, embedded online communities, and individual features. Securboration, Inc. has developed and prototyped the *Social Understanding and Reasoning Framework* (SURF) to find and classify individuals through their social media interaction. As of late 2016, SURF is at TRL 6 and the proof-of-concept is installed in the Tactical Information Fusion Laboratory at Aberdeen Proving Ground, MD. SURF has been applied to Twitter social networks and achieved 85% accuracy classifying two separate groups of individuals: ISIS Sympathizers and Arabic Businessmen.

SURF uses an innovative combination of social network analysis and machine learning that does not rely on language, but rather learned motifs (repeating patterns of subnetworks), resulting in over two hundred features prominent in ISIS related Twitter networks. As a result, ISIS sympathizers can be detected before they become true jihadist and go off the grid. This is a critical need, analogous to the Improvised Explosive Device (IED) challenges in Afghanistan and Iraq where the impetus for combatting IEDs shifted to interjecting to the '*left of the bang,*' before the device goes into the ground. This introduced a broad range of techniques, many based on human geography and social science, aimed to prevent neutral citizens from aligning with the insurgents. This early detection capability in SURF has a parallel '*left of jihad*' capability that fits in well with information tactics such as those being planned by the Center for Strategic Counterterrorism Communications.

SURF can also provide unprecedented capability for Intelligence Preparation of the Battlespace (IPB) to help identify ISIS sentiment in a particular area of operations, especially when fused with other intelligence sources. Specific SURF characteristics that enable these capabilities include: (i) language agnostic; successfully tested on Arabic, French, Spanish and symbol based languages, (ii) can work on Dark Networks (encrypted), (iii) extensible to classify other user types, e.g. religious leaders or Islamic cleric, CBRN scientist, etc., (iv) GOTs capability runs within Ozone Widget Framework as a thin client, and (v) automatically processes an overwhelming volume of social media information for the Warfighter.

B. Statistical Structural Health Monitoring in the Presence of Environmental Variability and Uncertainty
Investigator: Professor Luke Bornn, Harvard University, Young Investigator Program Award
Recipient: ARL Vehicle Technology Directorate (ARL-VTD)

The objective of this research is to develop real-time structural health monitoring (SHM) techniques through the derivation of mathematically rigorous statistical methods. Structural health monitoring encompasses identifying damage on all types of aerospace, civil and mechanical infrastructure systems based on changes in the measured dynamics response characteristics while the system is in operation. The PI has collaborated with Dr. Charles Farrar's group at the Los Alamos National Lab on SHM, with particular interest on the challenge to separate the operational and environmental variability phenomena. While rigorously derived techniques are often lacking in many SHM methods, Prof. Bornn introduced the switching vector auto-regressive model to the team and derived mathematically rigorous methods for applications to SHM real-time sensing techniques. This modeling capability was added to the SHMTools software, which is a library and application that was created by Dr. Farrar and his colleagues. The SHMTools software that included the PI's contribution was selected for a 2015 R&D 100 award.

Dr. Farrar and his colleagues teach a structural health monitoring short course for researchers and practitioners on the SHMTools software across the DoD. In Aberdeen, MD on March 21-23, 2016, Dr. Farrar's team trained

ARL researchers in their software. ARL's Vehicle Technology Directorate found this class extremely informative and very applicable to various research areas in their directorate, with potential application to Army vehicles that are susceptible to mechanical failure.

C. Computational Modeling of Epileptic Activity
Investigator: Professor William S. Anderson, Johns Hopkins School of Medicine, Single Investigator Award
Recipient: ARL Human Research and Engineering Directorate (ARL-HRED)

The objective of this research is to use computational modeling techniques coupled with novel human brain recordings in epilepsy patients to better understand the effects of cortical electrical stimulation. Specifically, the goals were to develop a calibrated computational model of normal and epileptic cortex using multi-compartment neuronal representations incorporating an effect of applied external electric fields and to compare the results obtained in simulation studies with recordings obtained from a new subdural grid design incorporating microwire recording elements during electrical stimulation.

The results of the research will improve the computational models of neural systems exposed to electric fields by including the activity of physiologic and pathophysiologic linked collections of neurons. This approach differs from previous approaches using passive excitable neuronal models that do not incorporate underlying network spiking behavior, upon which the electric field acts. The results of this project transitioned to ARL-HRED for further study as a potential means for investigating the relationships between blast-related neuronal injuries and large-scale brain network effects. These efforts strive towards identifying new robust biomarkers in iEEG/EEG that can aid in determining severity of the injury and monitoring the injury progression as well as in predicting the outcome. In addition, the network model will be useful in training and tuning of neuromodulation systems for suppression of pathological brain activity or for the aiding of memory disorders; currently the PI is investigating leveraged funding from DARPA for commercialization of these techniques.

D. Multiscale Modeling for Locally-Producible Cementitious Materials
Investigator: Professor Ram Mohan, North Carolina A&T, Partnership in Research Transition Award
Recipient: Army Corps of Engineers - Engineer Research and Development Center (ERDC)

The objective of this research is to evolve a multi-scale nano to continuum modeling methodology that links and transcends across the different length scales from the nano length scale material constituents to the macroscopic deformation and failure behavior through appropriate length scale models and their coupling that will impact the multi-scale modeling, design, and development of advanced cement material for force and materiel protection from direct, ballistic and shock threats in theater and for homeland security. Researchers at North Carolina Agricultural and Technical State University (NC A&T) have made mathematical advances that may provide a foundation for the creation of advanced high-performing materials for greater blast and ballistic protection to significantly improve base sustainability and readiness.

The researchers, in collaboration with U.S. Army Corps of Engineers' Engineer Research and Development Center (ERDC), University of Mississippi, Oxford, Sandia National Laboratories, and the National Institute of Standards and Technology (NIST), have developed computational models over a range of material features and scales of cement to address complex challenges in predicting mechanisms associated with deformation progression and failure of cement paste under varying loading conditions. Of particular significance is the model's potential for predicting performance of a wide variety of cement pastes, such as may be mixed from local materials during deployment. The research addresses a TRADOC Top 10 Warfighter Outcome in Individual Soldier Protection, and has resulted in 10 joint papers with ERDC, 8 joint papers with ARL-CISD, 8 Masters degrees, 4 PhDs, 3 Post Docs who secured academic appointments, and several invited and keynote presentations at international conferences.

V.   ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Subspace Methods for Massive and Messy Data
Professor Laura Balzano, University of Michigan, Single Investigator Award

Subspace tracking is an important modeling method for streaming data in video and computer vision, power grid monitoring, environmental sensing, and communications (among other applications). Professor Balzano's own state-of-the-art method, GROUSE, struggles with *ill-conditioned* data – i.e when there is a large dynamic range among the important signal components. One of the primary goals of this research has been to improve the performance on data with this characteristic.

More specifically, the goal for this new algorithm has been to achieve high accuracy on a subspace estimate using half as many iterations (data points) as standard GROUSE for data with condition number up to 1000 (i.e. the largest data points are 1000x magnitude of the smallest). The research team defines "high accuracy" depending on the noise level in each context, with a goal of getting to within 10x of the noise level (as generated in a simulated data context, and as estimated in real data).

To improve computational speed, the PI is developing yet another extension of the algorithm which tracks a low-rank subspace model over time. This algorithm can, for example, already model the background of an image as low-rank and then separate the foreground activity, even for images that are blurred or distorted by camera motion.

Another method being investigated by the PI is subspace clustering, which is a very common data analysis tool and is the model at the center of the PI's current research. The subspace clustering problem models each cluster as a low-dimensional subspace. State-of-the-art subspace clustering algorithms are unsupervised (no labeled points) and achieve best in class clustering error, but still above ~10-15% on benchmark datasets. It is anticipated that in FY17, the PI's goal is to drive this down with both new algorithms and active learning (labeling methods), achieving an improvement in recognition accuracy over the current state-of-the-art, as well as an error rate below 5% within a minimal number of queries when matching images to a fixed data base.

B. Nonlinear and Probabilistic Analysis with Frames
Professor Radu Balan, University of Maryland at College Park, Single Investigator Award

One of the main goals of this research is the advancement of novel mathematical techniques to analyze nonlinear phenomena, with particular interest in harmonic analysis of phase retrieval and quantum state tomography. The phase retrieval problem can be simply stated as recovery up to a global phase factor of an unknown vector from magnitudes of scalar products with a redundant set of vectors, and the quantum state tomography asks for recovery of a unit trace positive semi-definite symmetric form (from Hilbert-Schmidt scalar products with a set of self-adjoint operators). Other examples of nonlinear phenomena include X-Ray crystallography, speech recognition, deep learning, and non-convex optimization, all of which use nonlinear processing of incomplete information.

It is anticipated that in FY17, the PI will develop the theoretical methods that will create the phase retrievability property for quantum state tomography. Current approaches that solve the phase retrievability problem leverage methods from geometry, analysis, and statistics for systems with a finite-dimensional state space. These techniques are not able to handle infinite dimensional systems, which is a typical characteristic of quantum state spaces. A novel approach is required to create the phase retrievability property for infinite-dimensional systems. Furthermore, although the finite-dimensional problem has a built-in robustness, the estimation problem to derive the Lipschitz constants and Cramer-Rao lower bounds is still far from being solved. The challenge comes from a recent result that links the phase retrievability property to a NP hard problem. The understanding of existing

detection and estimation algorithms should provide insight into addressing the shortcoming of the existing algorithms and produce new methods and obtain efficient algorithms.

C. Warfighter Neuroendocrinology: Modeling stress response, PTSD and TBI
Professor Maria D'Orsogna, University of Michigan, Single Investigator Award

Stress related disorders affect multiple biological functions from endocrine system regulation to brain circuitry connectivity. Identifying the mechanisms that lead to the development of such disorders has been an active area of research, with a particular emphasis placed on understanding the dynamics of post-traumatic stress disorders (PTSD). Although many advances have been made, how PTSD emerges and evolves is still unclear. Experimental studies are challenged by incongruent diagnostic criteria and confounding treatment protocols. Although PTSD is often associated with low levels of cortisol, to date there is no reliable biological predictor or marker for PTSD and diagnoses are heavily reliant on self-reporting. Current treatments include psychotherapy and pharmacotherapy: it is not very clear how the two intervention methods inform each other and they are not always very successful. In part, these challenges are due to the lack of a comprehensive understanding of the biological processes and systems that are affected by PTSD and how they respond and interact with each other under stress.

The goal of this research is to develop and analyze a mathematical model that includes the relevant physiological features involved in stress response regulation. Specifically, PTSD-induces dysregulation of the hypothalamic-pituitary-adrenal (HPA) axis will be investigated using mathematical modeling. The mathematical model will provide a mechanistic description of how low basal cortisol levels observed in PTSD patients can arise from stress induced by traumatic experiences. This work will be useful as a way to study how the neuroendocrine system responds to various challenge tests used to assess HPA function in PTSD such as the administration of steroids such as Corticotropin Releasing Hormone (CRH), dexamethasone, and naloxone. Finally, results can guide the development of more quantitative tools to diagnose PTSD and as a way to distinguish its symptoms from other similar disorders.

It is anticipated that in FY17, the mathematical model will be expanded to include the limbic structures and brain stem areas that are coupled to the HPA and that are involved in stress response and related disorders at a higher level. Including these further systems will allow a more comprehensive model for the study of PTSD and other stress disorders. The current HPA model will also be used to evaluate intervention methods on PTSD patients and compare the results with data available in the literature. These methods include dexamethasone suppression tests, used to assess adrenal gland function by measuring how cortisol levels change in response to an injection of dexamethasone, naloxone stimulation tests that affect CRH expressions, and the direct administration of CRH and Adrenocorticotropic hormone.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Joseph Myers
Division Chief
Program Manager, Computational Mathematics
Program Manager (Acting), Probability and Statistics

Dr. Virginia Pasour
Program Manager, Biomathematics

Dr. Leonard (Jay) Wilkins
Program Manager, Modeling of Complex Systems

Dr. Andrew Vlasic
Contract Support, Probability and Statistics

B. Directorate Scientists

Dr. Randy Zachery
Director, Information Sciences Directorate

Dr. Bruce West
Senior Scientist, Information Sciences Directorate

Ms. Anna Mandulak
Contract Support

C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 9: MECHANICAL SCIENCES DIVISION

I. OVERVIEW

As described in CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication ARO in Review 2016 is to provide information on the programs and basic research supported by ARO in fiscal year 2016 (FY16), and ARO's mission to create basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Mechanical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY16.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mechanical Sciences Division supports research to uncover fundamental properties, principles, and processes involved in fluid flow, solid mechanics, chemically reacting flows, explosives and propellants, and the dynamics of complex systems of relevance to the Army and the DoD. More specifically, the Division supports basic research to uncover the relationships to: (i) contribute to and exploit recent developments in kinetics and reaction modeling, spray development and burning, (ii) gain an understanding of extraction and conversion of stored chemical energy, (iii) develop a fundamental understanding that spans from a material's configuration to a systems response to create revolutionary improvements through significant expansion of the mechanical design landscape used to optimizing systems, (iv) developing innovative frameworks for analyzing and shaping the physical mechanisms and dynamical interactions underlying the control of nonlinear behavior in extended dynamical systems; embodied and distributed sensing, actuation, and control for robotic manipulation and mobility; and nonlinear topological mechanics of novel meta-structures; and the interplay between statistical physics and control and learning, (v) provide the basis for novel systems that are able to adapt to their environment for optimal performance or new functionality, and (vi) develop a fundamental understanding of the fluid dynamics underlying Army systems to enable accurate prediction methodologies and significant performance improvement, especially with regard to unsteady separation and stall and vortex dominated flows. Fundamental investigations in the mechanical sciences research program are focused in the areas of solid mechanics; complex dynamics and systems; propulsion and energetics; and fluid dynamics. Special research areas have been continued in the Army-relevant areas of rotorcraft technology, projectile/missile aerodynamics, gun propulsion, diesel propulsion, energetic material hazards, mechanics of solids, impact and penetration, smart structures, and structural dynamics.

2. Potential Applications. Research managed by the Mechanical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO research in the mechanical sciences could provide understanding that leads to insensitive munitions, tailored yield munitions, enhanced soldier and system protection, novel robotic, propulsion, and novel flow control systems and enhanced rotorcraft lift systems. In addition, mechanical sciences research may ultimately improve Soldier mobility and effectiveness by enabling the implementation of renewable fuel sources and a new understanding of energetic materials with improved methods for ignition, detonation, and control.

3. Coordination with Other Divisions and Agencies. The primary interactions of this Division with other ARL S&T Campaigns are with the Sciences for Maneuver, Sciences for Lethality and Protection and Materials Research Campaigns. The Division also interacts with the U.S. Army Corps of Engineers (USACE), and various Army Research Development and Engineering Centers (RDECs), including the Aviation and Missile RDEC (AMRDEC), Natick Soldier RDEC (NSRDEC), and the Tank-Automotive RDEC (TARDEC). The Division facilitates the development of joint workshops and projects with Program Executive Office (PEO) Soldier and

the Army Medical Research and Materiel Command (MRMC). In addition, the Division often jointly manages research through co-funded efforts with the ARO Chemical Sciences, Materials Science, Mathematical Sciences, Computing Sciences, and Life Sciences Divisions. Strong coordination is also maintained with other Government agencies, such as the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the National Science Foundation (NSF), the National Aeronautics and Space Administration (NASA), the National Institute of Standards and Technology (NIST), and the Department of Energy (DoE). International research is also coordinated through the International Science and Technology (ITC) London and Pacific offices.

B. Program Areas

The Mechanical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of projects. In FY16, the Division managed research within these four Program Areas: (i) Solid Mechanics, (ii) Complex Dynamics and Systems, (iii) Propulsion and Energetics, and (iv) Fluid Dynamics. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Solid Mechanics. The goal of the Solid Mechanics Program is to investigate behavior of complex material systems under broad range of lading regimes in various environments, and to develop analytical and computational methods to characterize material models and to serve as physically-based tools for the quantitative prediction, control, and optimization of Army relevant material systems subjected to extreme battlefield environments. Army systems are frequently limited by material strength and failure resistance. Solid mechanics research plays a crucial role in the development of new materials, prediction of strength, toughness and potential damage development and failure of Army material systems, structures and individual protective equipment under extreme loading conditions such as impact or blast, and prolonged normal operating conditions. Research in analytical, computational and experimental solid mechanics forms the foundation of optimization tools to enhance performance while minimizing equipment weight, and its theories provide a strong link between the underlying mechanical behavior of solids and the resulting design and functionality of actual systems resulting in reduced development cost by minimizing the need for expensive field testing and it leads to novel ideas and concepts for revolutionary capabilities.

This Program Area is divided into two research Thrusts: (i) Investigation of mechanical behavior of complex material systems, and (ii) Development of analytical, computational and experimental methods capable to utilize material models in the analysis of extreme situations leading to damage and failure development. Current program efforts utilizing advanced multiscale computational and modeling techniques enabling detailed investigations of behavior of heterogeneous solids. The goal is to extend the design envelope of current and future Army structures, to develop predictive capability based on advanced ideas and understanding of material behavior across all relevant scales, to predict continuum and localized damage and failure initiation and development as it progresses across different scales, to give reliable estimates of the material limitations and useful life.

Research in this Program Area is focused on long-term, high risk goals that strive to develop the underpinnings for revolutionary advances in military systems. It is developing the methods needed to take advantage of recent advances in new materials fabrication and investigation technology, including nanotubes, nano-crystaline solids, and bio-inspired and hierarchical polymeric- and nano-composites. As a result of the long-term vision of the program, some future applications are not yet imagined while others will lead to the creation of ultra-lightweight, high strength materials for applications such as lightweight armor.

2. Complex Dynamics and Systems. The goal of the Complex Dynamics and Systems Program Area is to develop innovative frameworks for analyzing and shaping the physical mechanisms and dynamical interactions underlying the control of nonlinear behavior in extended dynamical systems; embodied and distributed sensing, actuation, and control for robotic manipulation and mobility; nonlinear topological mechanics of novel meta-structures; and the interplay between statistical physics and control and learning. In addition, the program has developed a set of Strategic Program Challenges (SPC) targeting questions relevant to the programmatic scientific focus areas deemed beyond the scope of single investigator awards. Current SPC topics include: (1)

Energetic Versatility of Muscles: Principles and Emulation, (2) Controlling Hyperelastic Matter, (3) Theory of Morphological Energetics, (4) Control and Creation of Critical Dynamics. , and (5) Nonlinear Topological Dynamics of Metastructures. The challenges emphasize high-risk, high-reward exploratory research to create breakthroughs, push science in truly novel directions, or to support mathematical abstractions and precise physical foundations for emerging technologies deemed likely to be of significant future Army and DoD impact. SPC's are developed by the program manager in close consultation with DoD researchers and university researchers.

The Complex Dynamics and Systems Program emphasizes fundamental understanding of the dynamics, both physical and information theoretic, of nonlinear and nonconservative systems as well as innovative scientific approaches for engineering and exploiting nonlinear and nonequilibrium physical and information theoretic dynamics for a broad range of future capabilities (e.g. novel energetic and entropic transduction, agile motion, and force generation). The program seeks to understand how information, momentum, energy, and entropy is directed, flows, and transforms in nonlinear systems due to interactions with the system's surroundings or within the system itself. Research efforts are not solely limited to descriptive understanding, however. Central to the mission of the program is the additional emphasis on pushing beyond descriptive understanding toward engineering and exploiting time-varying interactions, fluctuations, inertial dynamics, phase space structures, modal interplay and other nonlinearity in novel ways to enable the generation of useful work, agile motion, and engineered energetic and entropic transformations. The programmatic strategy is to foster mathematically sophisticated, interdisciplinary, and hypothesis-driven research to elucidate classical physics and analytical methods pertinent to the foundations of a broad spectrum of Army research areas including: mobility, power and energy, sensors, lethality, and trans-disciplinary network science.

3. Propulsion and Energetics. The goal of this Program Area is to explore and exploit recent developments in kinetics and reaction modeling, spray development and burning, and current knowledge of extraction and conversion of stored chemical energy to ultimately enable higher performance propulsion systems, improved combustion models for engine design, and higher energy density materials, insensitive materials, and tailored energy release rate. Research in propulsion and energetics supports the Army's need for higher performance propulsion systems. These systems must also provide reduced logistics burden (lower fuel/propellant usage) and longer life than today's systems. Fundamental to this area is the extraction of stored chemical energy and the conversion of that energy into useful work for vehicle and projectile propulsion. In view of the high temperature and pressure environments encountered in these combustion systems, it is important to advance the current understanding of fundamental processes for the development of predictive models as well as to advance the ability to make accurate, detailed measurements for the understanding of the dominant physical processes and the validation of those models. Thus, research in this area is characterized by a focus on high pressure, high temperature combustion processes, in both gas and condensed phases, and on the peculiarities of combustion behavior in systems of Army interest.

To accomplish these goals, the Propulsion and Energetics Program Area has two research Thrusts: (i) Hydrocarbon Combustion, and (ii) Energetics. The goal of the Hydrocarbon Combustion Thrust is to develop novel, predictive models for reacting systems especially for heavy hydrocarbon fuels, surrogate fuel development, and research into sprays and flames, especially ignition in high pressure low temperature environments. In addition the Energetics Thrust focuses on novel material performance via materials design and development and materials characterization, and investigations (theoretical, modeling and experimental) into understanding material sensitivity (thermal and mechanical).

4. Fluid Dynamics. Fluid dynamics plays a critical role in many Army operational capabilities. Significant challenges exist for accurate and efficient prediction of flow physics critical for improved performance and future advanced capability. Army platforms are often dominated by flows with high degrees of unsteadiness, turbulence, numerous and widely separated spatio-temporal scales, and geometrical complexity of solid or flexible boundaries. In order to gain the necessary physical insight to enable future capabilities spanning Army vehicles, munitions, medical devices, and logistics, the Fluid Dynamics program seeks to support basic research investigations of fundamental and novel flow physics. In view of the nonlinear and high-dimensional character of the governing equations, revolutionary advances in fluid dynamics research tools are also of great interest; advanced experimental methods, sophisticated computational techniques and breakthrough theoretical advances will be critical for gaining the required fundamental understanding.

Operating conditions for many Army platforms are characterized by flows featuring unsteadiness, nonlinear interactions, turbulence, three-dimensionality and flow separation. All efforts in this thrust area require novel and aggressive strategies for examination of the interplay between disparate spatio-temporal scales, inclusion of physically significant sources of three-dimensionality, and characterization of the role of flow instabilities and nonlinear interactions across a range of appropriate Mach and Reynolds numbers. Shortcomings in understanding the details of unsteady flow separation, reverse flow phenomena, and dynamic stall continue to limit the capabilities of Army rotorcraft vehicle platforms. While much progress has been made towards unraveling these details, it has become apparent that revolutionary advances are unlikely if the full complexity of the physics is not considered. Finally, many Army relevant flows are governed by strong nonlinearities and turbulent behaviors. Historically, many analysis tools developed for linear dynamics have been applied to gain understanding of flow behaviors. While local insights can be gained through applications of these methods, the ability to provide global understanding of the evolution of flows requires new approaches that are capable of dealing directly with inherent nonlinearities.

C. Research Investment

The total funds managed by the ARO Mechanical Sciences Division for FY16 were $16.6 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $7.1 million and $1.1 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $6.0 million to projects managed by the Division. The Division also managed $1.3 million of Defense Advanced Research Projects Agency (DARPA) programs. In addition, $0.9 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.4 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY16 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY16 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY16, the Division awarded 25 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Josette Bellan, California Institute of Technology; *A Unified Modeling Approach for Simulating Thermodynamic Phase Transformations during Turbulent Mixing and Combustion of Diesel*

- Professor Erik Bollt, Clarkson University; *Criticality and Information Fragility in Complex Systems*

- Professor Joshua Bongard, University of Vermont; *Morphological Plasticity for the Design, Control and Deployment of Complex Engineering Systems*

- Professor Oana Cazacu, University of Florida - Gainesville; *Uncovering The Cause of Ratcheting and Low-Cycle Fatigue*

- Professor Itai Cohen, Cornell University; *Engineering Dynamic Skin*

- Professor Maria Fonoberova, AIMdyn, Inc; *Koopman Mode Decomposition: Revisiting the Route to Turbulence*

- Professor Seth Fraden, Brandeis University; *Control of Hyperplastic Chemomechanical Materials*

- Professor Roger Hanlon, Marine Biological Laboratory; *Mechanisms And Tradeoffs of Peripheral and Central Control of Dynamic Skin Patterning in Cephalopods*

- Professor David Henann, Brown University; *Nonlinear Constitutive Modeling of Viscoelastic Foams*

- Professor Yiguang Ju, Princeton University; *Multiscale and Correlated Dynamic Adaptive Chemistry and Transport Modeling of Ignition and Flame Regimes of Stratified Fuel Mixtures*

- Professor Eva Kanso, University of Southern California; *Active and Passive Actuation of Bio-Inspired Locomotory Systems*

- Professor Robert Lipton, Louisiana State University and A&M College; *Mathematical and Multi-Scale Foundations of Nonlocal Modeling*

- Professor Kevin Lyons, North Carolina State University; *Propulsion and Energetics Investigations of Turbulent Lifted Flame Stabilization in Heated and Vitiated Coflows*

- Professor Carmel Majidi, Carnegie Mellon University; *Nonlinear Dynamics and Distributed Control for Soft Robot Locomotion*

- Professor Todd Murphey, Northwestern University Evanston Campus; *Transforming Terrestrial Agility At All Scales*
- Professor Venkateswaran Narayanaswamy, North Carolina State University; *Investigation of Shock Interactions with Distorted Boundary Layers for Precision Munition Applications*
- Professor Hiroaki Nishikawa, National Institute of Aerospace Associates; *Hyperbolic Reconstructed-Discontinuous-Galerkin Method for Accurate Unsteady Viscous Simulations on Unstructured Grids*
- Professor Oliver O'Reilly, University of California - Berkeley; *Nonlinear Dynamics and Distributed Control for Soft Robot Locomotion*
- Professor Derek Paley, University of Maryland - College Park; *Nonlinear Dynamics and Distributed Control for Soft Robot Locomotion*
- Professor Steve Presse, Indiana University - Purdue University at Indianapolis; *Multi-Dimensional and Dissipative Dynamical Systems: Maximum Entropy as a Principle for Modeling Dynamics and Emergent Phenomena in Complex Systems*
- Professor Kalyanasundaram Seshadri, University of California - San Diego; *Autoignition and Combustion of JP-8, Reference Fuels and Surrogates in Nonuniform Flows at Elevated Pressures*
- Professor Henry Sodano, University of Michigan - Ann Arbor; *Mechanics of Nanowire Interfaces Across Strain Rates*
- Professor Hareesh Tippur, Auburn University; *Dynamics of Crack-Interface Interaction in Layered Transparencies: An Experimental Investigation using Novel Optical Techniques*
- Professor Barry Trimmer, Tufts University; *Dynamic Tuning of Instabilities for High Power Movements in Deformable Structures*
- Professor Minami Yoda, Georgia Tech Research Corporation; *A Fundamental Study of Electrokinetic Instabilities to Manipulate and Self-Assemble Nano- and Microparticles*

2. Short Term Innovative Research (STIR) Program. In FY16, the Division awarded three new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Giuseppe Buscarnera, Northwestern University Evanston Campus; *Modeling Rate-Dependent Dissipation in Granular Solids via Continuum Thermodynamics*
- Professor Chung Law, Princeton University; *Droplet-Wall/Film Impact in IC Engine Applications*
- Professor Stephen Tse, Rutgers, The State University of New Jersey - New Brunswick; *Ignition by Electric Spark Discharges Triggered by the Fuel/Energetic Aerosol Itself*

3. Young Investigator Program (YIP). In FY16, the Division awarded one new YIP project to drive fundamental research in areas relevant to the current and future Army. The following PI and corresponding organization were recipients of the new-start YIP award.

- Professor Samuel Burden, University of Washington; *Predictive Models for Sensorimotor Control of Legged Locomotion*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY16 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *A Workshop for High-Fidelity Simulation Based Virtual Testing of Composite Materials and Structures*; Coral Gables, FL; 19-20 April 2016
- *2016 Energetic Materials - Gordon Research Conference*; Stowe, VT; 5-10 June 2016
- *Eleventh International Symposium on Special Topics in Chemical Propulsion: Recent Progress in Energetic Materials and Chemical Propulsion, Istanbul, Turkey, June 12-16, 2016*; Istanbul, Turkey; 12-16 June 2016
- *IUTAM Symposium on Integrated Computational Structure_ Material Modeling of Deformation and Failure Under Extreme Conditions*; Baltimore, MD; 19-22 June 2016
- *2016 Princeton-CEFRC-CI Summer School on Combustion*; Princeton, NJ; 19-24 June 2016

- *Workshop on Information Engines at the Frontiers of Nanoscale Thermodynamics*; Telluride, CO; 23 June – 1 July 2016

5. Special Programs. In FY16, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded seven new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES. These awards constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Nanoscale Control, Computing, and Communication Far-from-Equilibrium. One MURI in this topic area began in FY13. The team is led by Professor James Crutchfield of the University of California at Davis. The objective of this MURI is to develop fundamental understanding to enable new synthetic nanoscale systems capable of behaving as information engines, performing tasks that involve the manipulation of both information and energy. Ultimately, a unified framework for understanding, designing, and implementing information-processing engines will be developed by a team of experts in information processing by dynamical systems, nonequilibrium thermodynamics, control theory, and nanoscale devices to search for and articulate the basic principles underlying the manipulation of information and energy by synthetic nanoscale systems. Theoretical predictions will be empirically validated in experimental nanoscale devices.

This research will enable new capabilities to (i) quantify the intrinsic computation in nanoscale thermodynamic systems, (ii) to produce a thermodynamic theory for control and optimization of out-of-equilibrium nanoscale processes, and (iii) to accomplish experimental validation of the resulting thermodynamic principles of optimization and control of molecular agents. The results will provide a scientific foundation for future nanoscale devices with groundbreaking capabilities, ranging from efficient computation on microscopic substrates to the generation of directed motion. In the long term, this research may enable devices that can coordinate the molecular assembly of materials and novel substrates for information processing on radically smaller and faster scales. This research may lead to a new generation of faster, cheaper, and more energy efficient computing devices capable of manipulating large-scale, complex data structures, as well as self-organizing nanoscale motors capable of interfacing with the physical world with maximum power and efficiency.

2. New Theoretical and Experimental Methods for Predicting Fundamental Mechanisms of Complex Chemical Processes. This MURI began in FY14 and was awarded to a team led by Professor Donald Thompson of the University of Missouri, Columbia. The objective of this MURI is to develop new approaches to predictive models for complex, reacting systems. It will develop supporting fundamental theory, perform supporting experiments, and validate resultant models and methods. The goal is to develop computationally efficient, predictive, accurate, robust methods to predict the molecular energy hypersurface, as well as relevant pathways and bifurcation topology for reacting coordinates.

The effort will accomplish the objectives via a comprehensive research program that will design efficient methods to predict and control the behavior of complex chemical reactions, such as combustion. Complexity is the salient challenge facing modern physical chemistry, and the proposed research will yield fundamental new methods to directly address the complexity of chemical reactions - from ab initio principles to the collective evolution of chemical populations. The research program is based on two ideas: (i) It is not necessary to describe or even know all the details, only those directly involved in the relevant pathway(s) from reactants to products, and (ii) it is essential to understand the role of fluctuations in the reaction rate, such as those that can be induced by the energetic environment and the many intermediates in combustion processes. The robust and accurate methods developed will determine the critical, emergent behaviors of complex overall reactions in non-equilibrium environments. They will accurately describe how a set of reactants undergoes sequential, branching reactions, passing through many transition states and transient species, to reach a final set of stable products. To

gain an understanding of the role of fluctuations in reaction rates far from equilibrium, the researchers will focus on extracting information from the detailed dynamics of molecular species that are responsible for the fluctuations and, ultimately, the limits of traditional chemical kinetics. A synergistic approach will be undertaken for these overarching challenges that integrates the full range of rigorous fundamental theoretical methods. The specific objectives of the project leverage the complexity of kinetic phenomena, which are typically nonlinear, stochastic, multi-dimensional, strongly coupled, and can persist far from equilibrium by extreme variations in intensive properties. Some of the sub-objectives will be to: (1) Fully leverage the predictive capabilities of state-of-the-art electronic structure theory. (2) Gain a better understanding of how complex chemistry occurs at a microscopic level over wide ranges of temperature and pressure. (3) Identify and control relevant dynamical variables that can be probed experimentally. (4) Elucidate the role of statistical fluctuations in energy and matter on chemistry by analyzing the underlying nonlinear dynamics and reaction networks. (5) Design tractable theoretical and computational methods with immediate experimental links and reduced dimensionality without diminishing predictive capabilities. (6) Formulate connections among complexity theories, nonlinear dynamics, network theory, and chemistry. (7) Seek kinetic control of chemical and energetic phenomena on a macroscopic (rather than microscopic) level using nonlinear dynamics, optimal control, large deviations, and network theory.

3. Emulating the Principles of Impulsive Biological Force Generation. This MURI began in FY15 and was awarded to a team led by Professor Sheila Patek of Duke University. The objective of this MURI is to establish a unified theory for understanding biological and engineered impulsive systems. The MURI team will approach the objective using a thermodynamic framework linked to impulsive performance. This will require integrating mathematical analysis, tests of biological impulsive systems, and synthesis of impulsive materials and mechanisms. The thermodynamic framework consists of five phases: (1) chemical energy conversion in cellular biological systems that potentially circumvent the force-velocity tradeoffs of actin-myosin muscle mechanisms; (2) actuation tuned to spring loading through novel engineering implementations and informed by analyses of muscular and cellular thermodynamics; (3) potential energy storage through a diversity of biological materials, scales and geometries to inform synthetic elastic design; (4) rapid conversion from potential to kinetic energy (power amplification) – a defining feature of impulsive systems – through analyses of rate-dependence in biological materials/geometries, the mechanics of biological linkages and latches, and their directed synthesis into novel impulsive designs; and, (5) environment-system interactions through rigorous tests of the effects of environmental substrates and geometries, internal dissipation and reset mechanisms for repeated use and mitigation of failure due to environmental forces. This research effort will lay the foundations for scalable methods for generating forces for future actuation and energy storing structures and materials.

4. Multi-modal Energy Flow at Atomically Engineered Interfaces. This MURI began in FY16 and was awarded to a team led by Professor Jon Paul Maria of the North Carolina State University. The objective of this MURI is to bring chemistry, materials, surface science, electrochemistry, and physics together to characterize and understand short time-frame sub-nanoscale non-equilibrium phenomenon at and across materials interfaces, especially the flow, redistribution and partition of energy near the interface by devising and applying novel experimental, theoretical, and simulation approaches. The MURI team approach will be to explore, identify, and define multiple mechanisms of energy transfer/transduction at precision-engineered interfaces. Material systems that support energy transfer through lattice/molecular vibrations, plasmon-electron coupling, and chemical reactions will be studied. The synthesis, measurement, and modeling activities are co-designed to promote extreme-non-equilibrium excitations within nano-scale geometries; to observe in situ picosecond to microsecond property responses using newly developed methods; to inform new theoretical models; and to enable accurate multiscale prediction. The plan of work explores a simple, overarching, and materials-generic hypothesis: function and failure in advanced functional materials are overwhelmingly affiliated with interfaces, where the underlying mechanisms (desirable and undesirable) are regulated by or related to energy transfer/ transduction among inhomogeneous boundaries. Observing and understanding the local processes over multiple time and length scales will improve existing and design new materials systems, and to predict their performance.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY16.

D. Small Business Technology Transfer (STTR) – New Starts

No new starts were initiated in FY16.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY16, the Division managed one new ARO (Core) HBCU/MI projects and two new REP awards in addition to active projects continuing from prior years. Refer to CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY16.

G. Defense University Research Instrumentation Program (DURIP)

As described in CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY16, the Division managed nine new DURIP projects, totaling $1.8 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Reactive Material Structures Program

The Mechanical Sciences Division serves as the agent for the DARPA-sponsored Reactive Material Structures (RMS) program. This program was initiated in FY08 with an objective to develop and demonstrate materials/material systems that can serve as reactive high strength structural materials (*i.e.*, be able to withstand high stresses and can also be controllably stimulated to produce substantial blast energy). In FY13, Phase II of the program began, which continued and expanded research efforts. Research is investigating innovative approaches that enable revolutionary advances in science, technology, and materials system performance. The Mechanical Sciences Division currently co-manages projects in this program seeking to explore rapid fracture and pulverization of the material, dispersion of the particles, and material ignition and burning, all while achieving strength, density and energy content metrics. The vision of the RMS program is to be able to replace the inert structural materials currently used in munition cases with reactive material structures that provide both structural integrity and energy within the same material system along with the ability to rapidly release the energy upon demand.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Mechanical Sciences Division.

A. Mesoscale Dislocation Mechanics Approach to Dynamically Propagating Shear Bands
Professor Amit Acharya, Carnegie Mellon University, Single Investigator Award

The objective of this project is to develop a computational tool for modeling damage due to propagating localized bands of plastic deformation in metals, in particular shear bands, under both high temperature and room temperature conditions. Shear banding in metals has been studied by using well-established elastic and bulk inelastic response functions. However, these responses by themselves along with the conventional theory of elasto-viscoplastic materials are incapable of representing the existence and the propagation of a deformation band tip curve that propagates in the material thereby extending the thin layer of the deformation band, as overwhelmingly observed in experiment. Developing an appropriate theory that overcomes this fundamental limitation of conventional theory and its implementation and validation is the primary goal of the project.

During FY16, two finite element implementations of the full finite deformation theory of Mesoscale Field Dislocation Mechanics (MFDM) have been developed, both adapted to parallel computation. One implementation is for quasi-static deformations and the other for the fully dynamic scenario. Both implementations have been extensively verified, with results of some selected physically meaningful verification tests shown below. The functionality obtained from their combination is really suited for parallel computations and large scale numerical simulations. The developed computational scheme is based on: (1) Extended small-deformation (M)FDM FEM implementation which includes balance of energy, thus providing the equation for evolution of temperature. (2) Developing an efficient FEM implementation for finite deformation (M)FDM theory. This includes accounting for (a) finite anisotropic elasticity (that accounts for pressure dependence of second-order elastic moduli), (b) the wealth of classical mechanics of materials knowledge (both constitutive and modeling) related to accounting for rate-dependence and thermal softening of the strength of the material, (c) coupling with the energy equation that provides the equation of temperature evolution and interaction of mechanical response with thermal softening and heat conduction. (3) Validation of developed computational model with experimental results for adiabatic shear banding.

The developed code employs the Message Passing Interface (MPI), thus enabling it to do parallel processing and is scalable to hundreds and thousands of processors. This accomplishment stands as a first computational implementation of a partial differential equation based model of the mechanics of dislocations at finite deformations in the whole literature, including time- dependent behavior in total deformation and dislocation plasticity.

For the implementation with material inertia, an alternate, equivalent formulation is utilized that is better adapted to the needs of a fully dynamic algorithm which resolves time scales related to the elastic wave speed of the material. Constitutive equations for single crystal as well as polycrystal response have been incorporated where finite elasticity, rate dependence in plastic response, material-strength evolution including thermal softening have all been accounted for with, currently, adiabatic increase of temperature due to plastic deformation. Also, the finite element formulation accounts for volumetric locking that needs to be accommodated for accurate computations of total deformation at large plastic strains. To maintain computational efficiency, one may alternate between solving the equations of rate equilibrium and the actual equilibrium equations for force balance. This allows avoiding a fully implicit scheme which would be impractical.

The verification of the developed numerical model were conducted using the following tests: (1) Burgers vector constancy under elastic deformation, (2) invariance of dislocation stress field after cyclic elastic deformation vis-à-vis volumetric locking formulation, (3) prediction of shear banding via kinematics; evolving temperature distribution in a shear band, and (4) development of heterogeneity under nominally homogeneous deformation (see FIGURE 1).
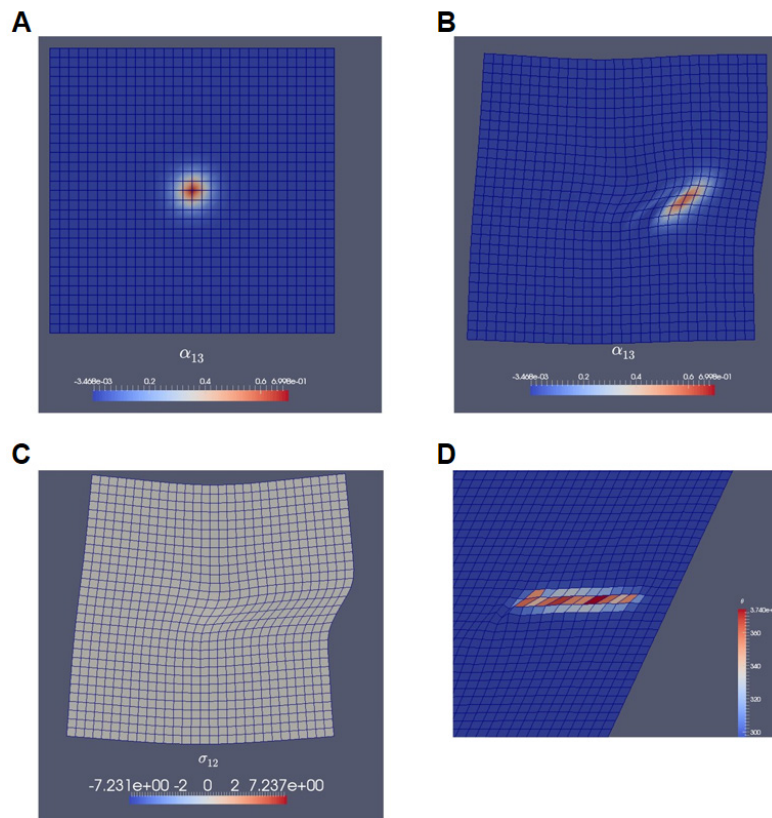
FIGURE 1

Verification of the developed numerical model. (**A**) Body with a single straight edge superdislocation. (**B**) The superdislocation moves due to an applied shear stress on the body. (**C**) On exit of the superdislocation, the body is left in a stress free but deformed state, with a shear band being produced along the path of motion of the superdislocation core. The motion of the core under a shear stress and the shear band produced is a pure kinematic consequence of the theory, and not a constitutive one. (**D**) Heterogeneous temperature profile produced along an extending shear band in dynamic deformation (different simulation from the other three results in this figure). The nature of the temperature heterogeneity has some preliminary similarity with experimental results of [GRR01b] which is encouraging, while much more remains to be done.

B. Validated Predictive Modeling of Engineered Cellulose Materials
Professor Sinan Keten, Northwestern University, Single Investigator Award

The objective of this research is to establish the theoretical link between cellulose nanocrystal (CNC) interface characteristics and the fracture toughness of engineered CNC neat films and nanocomposites. To accomplish the set objective, a meso-scale model was built to study the fracture behavior of neat films, using atomistically-informed coarse-grained models. This study reveals the size-dependence of the fracture behavior of layered CNC nanomaterials and contrast this with existing micromechanics theories such as shear-lag models.

The researchers investigated interfacial mechanics of nacre-inspired layered nanoparticle-PMMA layered nanocomposite systems by performing pull-out simulations using a coarse-grained molecular dynamics (CG-MD) approach to uncover two different deformation and failure mechanisms. These two mechanisms which greatly influence the toughness and energy dissipation of the system are: pull-out failure, which occurs along the particle–PMMA interface, and yielding failure, which occur within the nanofillers. Multi-layer graphene (MLG) and nanocellulose are examples. Taking graphene as a simpler model than CNCs, a theoretical model validated by the simulation data was built to determine the critical number of layers (Ncr) of graphene that governs the mode of failures as a function of MLG length and graphene- polymer interfacial interactions. In FY16, it was found that when the number of graphene layers is less than the critical number, (N ≤ Ncr), significant energy dissipation is observed via yielding failure mode, a direct result of the staggered arrangement of MLG. This staggered architecture allows sliding between graphene sheets, resulting in higher toughness compared to that of pull-out failure mode when N > Ncr. It was also found that increasing the system length L and the interfacial

interaction strength εgp between the layers will enhance the energy dissipation of the nanocomposite, which is a direct result of the nacre-like layer-by-layer arrangement of hard and soft phases (see FIGURE 2).
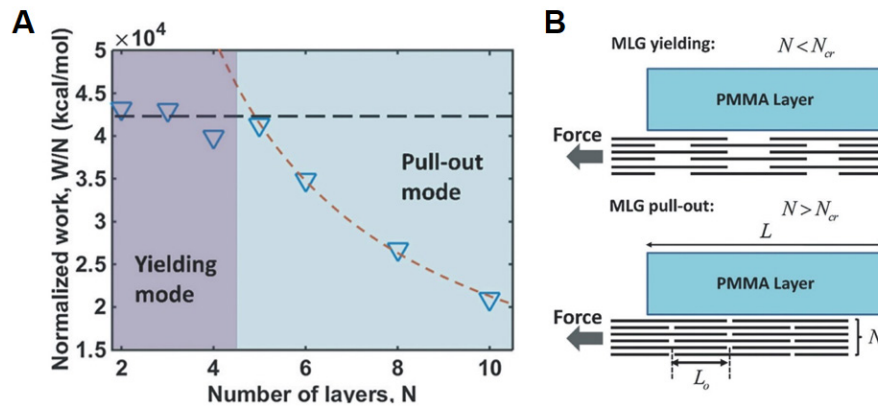

FIGURE 2

Failure behavior of layered nanocomposites. When a multi-layer filler like graphene or CNCs are employed in polymer matrices, failure mechanism depends on the number of layers and interfacial chemistry. Specifically, there exists a critical number of layers below which failure will be ductile, as it will facilitate yielding of the fillers, as opposed to simple pull-out of the fillers. This is contrary to most composites, where pull-out is considered a relatively dissipative failure mechanism, but for layered nanofillers yielding of the fillers further increases work to fracture due to creation of more failure surfaces.

Further, moisture is known to be an important parameter in dictating the mechanical properties of CNC based layered nanocomposites, where water trapped between layers can lower strength, and also cause a drying creep type of phenomena more commonly associated with cementitious materials (known as the Pickett effect). A coarse-grained model based on the dissipative particle dynamics approach was built where the behavior of nanoconfined water and its impact on the creep behavior of layered materials was investigated in a generic fashion. The researchers investigated how creep deformations in a slit pore are accelerated by the motion of water due to drying forces; it was found that the drying that drives water flow in the nanopores lowers both the activation energy of pore walls sliding past one another and the apparent viscosity of confined water molecules. This behavior and related shear-thinning phenomena can be captured with an analytical Arrhenius relationship accounting for the role of water flow in overcoming the energy barriers. Notably, using this model and simulation results it was demonstrated that the drying creep strain is not linearly dependent on the applied creep stress at the nanopore level. The findings establish the scaling relationships that explain how the creep driving force, drying force and fluid properties (e.g. viscosity under nanoconfinement) are related. Thus, the nanoscale origins of the Pickett effect were established which in turn provide strategies for minimizing the additional displacements arising from this effect.

Similarly, the mechanical behavior of nanoconfined polymers was investigated showing that significant stiffening can be attained when the interfacial energy between filler layers and polymers are large. This effect is more dramatic when the polymers have low internal cohesive energy, and also when the polymer layer thickness is relatively small. It was demonstrated that CNCs exhibit similar properties to MLG in terms of mechanical properties and layered structure, and thus a direct connection exists between these systems. This study ascertained the importance of surface chemistry of CNCs to achieve greater benefits from nanoconfinement of polymers between fillers.

Using a thin film nanocomposite analogy, the described methodology was used for predicting glass-transition temperature (T_g) in CNC-PMMA nanocomposites. It was discovered that increasing the volume fraction of CNCs results in nanoconfinement effects which lead to an appreciation of the composite Tg. Provided that strong interfacial interactions are achieved, as in the case of TEMPO- mediated surface modifications then promote hydrogen bonding. The upper and lower bounds of shifts in Tg were predicted by fully accounting for nanoconfinement and interfacial properties, providing new insight into tuning these aspects in nanocomposite design. This multiscale framework explains recent experiments and breaks new ground in predicting, without any empirical parameters, key structure−property relationships for nanocomposites (see FIGURE 3).

The analytical relations developed here describe the shear and tensile failure of the interfaces between Iβ CNCs, providing new insight into factors governing the mechanical behavior of neat films. Analytical models to describe the energy landscapes are developed using energy scaling relations for van der Waals surfaces in combination with a modification of the Prandtl–Tomlinson model for atomic friction. These simulations paved the way for tailoring hierarchical CNC materials.
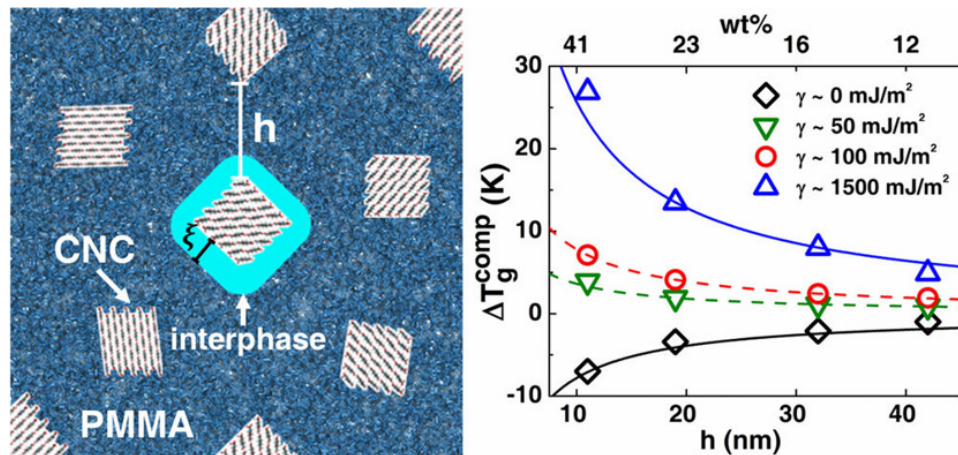

FIGURE 3

Predicting the glass-transition shifts in CNC-PMMA nanocomposites using a thin-film nanocomposite analogy. CNC surface modifications that improve adhesion to the matrix can lead to increases in the glass-transition temperature (T_g)at relatively high wt %, whereas lowering surface interactions with the matrix typically leads to lowering T_g.

C. Evolutionary Mechanics of Impulsive Systems – Guiding Scalable Synthetic Design
Professor Sheila Patek, Duke University, MURI Award

The goal of this research is to develop a program to discover underlying principles by which impulsive biological systems achieve a trio of capabilities that exceed current engineering performance: (1) extraordinary accelerations and speeds that (2) can be continuously fueled through metabolic processes and (3) are used repeatedly with minimal performance costs throughout the life of the organism. However, biological systems also face constraints that engineered systems have overcome; for example, engineered impulsive systems span a larger size range than the exclusively small biological impulsive systems. Similarly, engineered materials have outstanding capabilities for rate-dependent behavior, but the biological mechanisms for achieving asymmetric energy flow have yet to be analyzed. Underlying the rich array of capabilities and constraints that merge and delineate engineered and biological impulsive systems is a pressing need for a new field that articulates, through experiment, synthesis and theory, the fundamental principles of impulsive mechanisms. Therefore, the integrated approach of this research is to examine the capabilities and limitations of both biological and engineered systems while establishing the unifying mathematics and physics that explain these systems via the following four objectives. (1) Mathematically define and fabricate the units of impulsive propulsion. (2) Resolve the scaling limits and efficiency of energy storage in biological versus engineered systems. (3) Define the material, mechanical and structural basis for the inherent asymmetry in energy flow of impulsive systems. (4) Test the role of environment-system interactions in energy conversion, scaling and dissipation for failure reduction.

This program had several significant research contributions in FY16 concerning these four objectives. For Objective 1, the research team completed a team paper that establishes the three critical areas for analysis and that includes example mathematical models for each arena (motor, energy storage, latching) and began preliminary testing of 3D printing systems actuated with magnets to create impulsive models. For Objective 2, the research team established two cellular impulsive systems and an experimental setup to measure performance and mechanisms (including live-cell fluorescence high speed imaging, trigger protocols, microfabrication of flow chambers, and quantification of behavior), discovered novel cellular jumping behavior and used both experimental methods and mathematical modeling to assess environmental dissipation, power density and

behavioral function. For Objective 3, the research team discovered that combined effects of elasto-capillary force and phase-transition instability could be applied to a responsive-polymer-based micro-actuator to generate high elongation and high speed motion; designed and built novel instrument to perform large strain, high strain-rate material testing: Power Amplified Dynamic Mechanical Analyzer; established a new framework of latch definitions, classification, and metrics in impulsive systems; and built and tested physical models of mantis shrimp and trap-jaw ants and used variants of these models explore a range of actuation, energy storage and release systems. The variation of the components were used to test initial scaling and performance hypotheses and how their interactions can enhance impulsive performance (see FIGURE 4). For Objective 4 the research team built a new device to measure environmental energy return and its effect on power output in biological systems; collected data on jumping organisms that establishes that only a small percent (>15%) energetic recovery and that suggests constraints on biological impulsive systems for environmental tuning; and deployed physical models of impulsive organisms in different physical environments to assess environmental energy dissipation and its effect on impulsive performance.
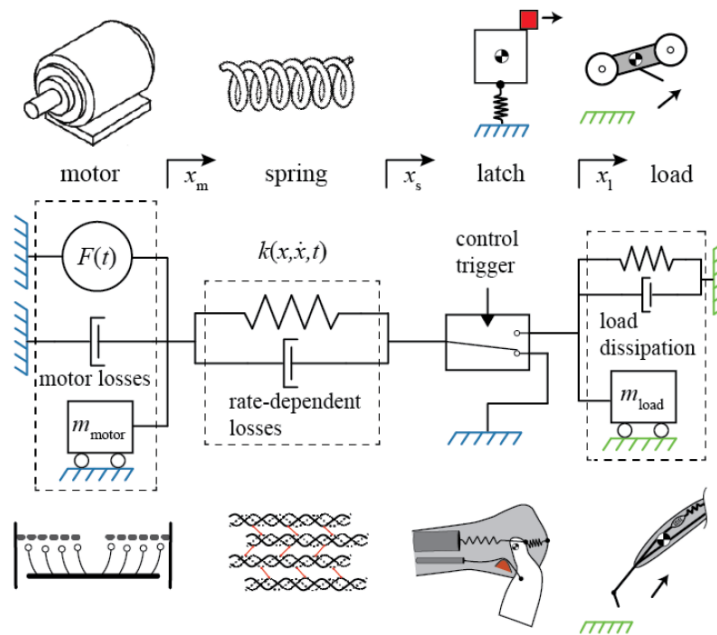

FIGURE 4

Framework for Understanding Impulsive Systems. An impulsive system can be conceptually and mathematically separated into lumped-parameter elements. Research focuses on systems with four fundamental components: motor/muscle, a potential energy storage mechanism, a latch with a controllable trigger, and a load. Understanding the impact of conservative and non-conservative forces on each component is critical to understanding the performance of the system as a whole. The top panel shows engineered components and the bottom panel shows biological components of impulsive systems.

D. An Investigation on Structures of Premixed Flames in High Intensity Turbulent Flow
Professor Ahsan Choudhuri, University of Texas - El Paso, HBCU/MSI – REP Award

The objective of this research is to study the structures of backward-facing step stabilized premixed flames in high turbulence flow, with the aid of KHz-level optical and laser diagnosis technology. This research is conducted cooperatively between the Center for Space Exploration Technology Research (cSETR) at the University of Texas at El Paso and Princeton University's Advanced Combustion and Propulsion Research Lab. The use of such technology will allow the team to generate experimental data at compressible and high Reynolds number conditions to address the following research questions: 1) What are the characteristics of premixed flame structures at a compressible and high intensity turbulent combustion? 2) What is the limit of regime boundaries at this condition? and 3) What scales affect the characteristics of the flame zone?

In FY16, the experimental setup has been tested under reacting flow. Testing was conducted at three different flow rates corresponding to Re= 15000, 32000, 64000, A turbulence generating grid with a blockage ratio (BR)

of 61% BR – 3 mm hole diameter perforated plates were used for the test runs. Images of reacting flow inside of the combustion chamber corresponding to the three different flow rates are shown in FIGURE 5. The PIV system was utilized to analyze the fluid flow characteristics inside the combustion chamber at three different flow rates (Re=15000, Re=32000, Re=64000) at a trigger rate of 10 kHz. A 56 mm x 42 mm interrogation area was used for the PIV and OH-PLIF analyses. The PIV interrogation area was located immediately downstream of the step expansion in the combustion chamber.
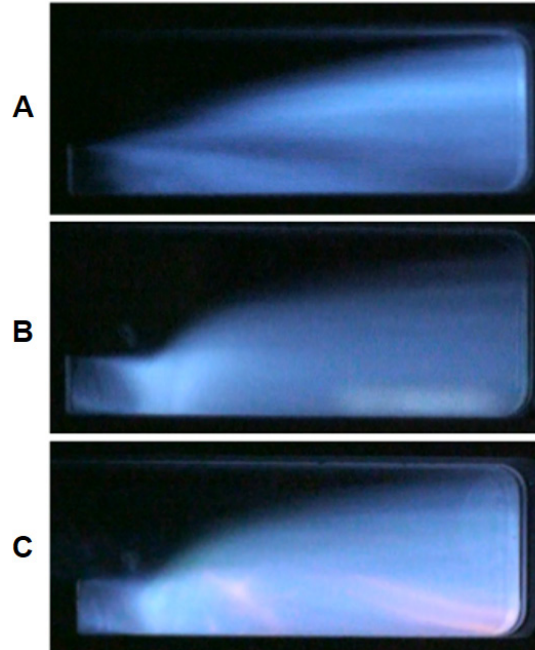
FIGURE 5

Instantaneous images of reacting flow at (**A**) Re=15,000, (**B**) Re=32,000, and (**C**) Re=64,000, with a trigger rate of 10 kHz.

FIGURE 6 shows three different analysis used for the three different Reynolds number conditions tested. OH-PLIF at 283nm excitation was used to map flame front characteristics at the three different flow rates (Re=15000, Re=32000, Re=64000) at a rate of 10 kHz. MATLAB software is used to post-process OH-PLIF images by isolating the edge of the burned and unburned gas to show the flame front location. Average OH-PLIF images were used to determine flame front location. Horizontal interrogation lines were placed along the flame front edge. Pixel intensity at these lines was plotted. A 20% threshold was used to determine the location of the flame front based on pixel intensity. According to flow parameters obtained from PIV imaging and calculated flame parameters (flame speed and flame thickness), the current operating flame regime for the combustor testing lies in the corrugated-flame and the thin reaction zones regimes. The ranges of Da, Ka, ReT, u', SL, for the test series conducted were determined (see FIGURE 7).
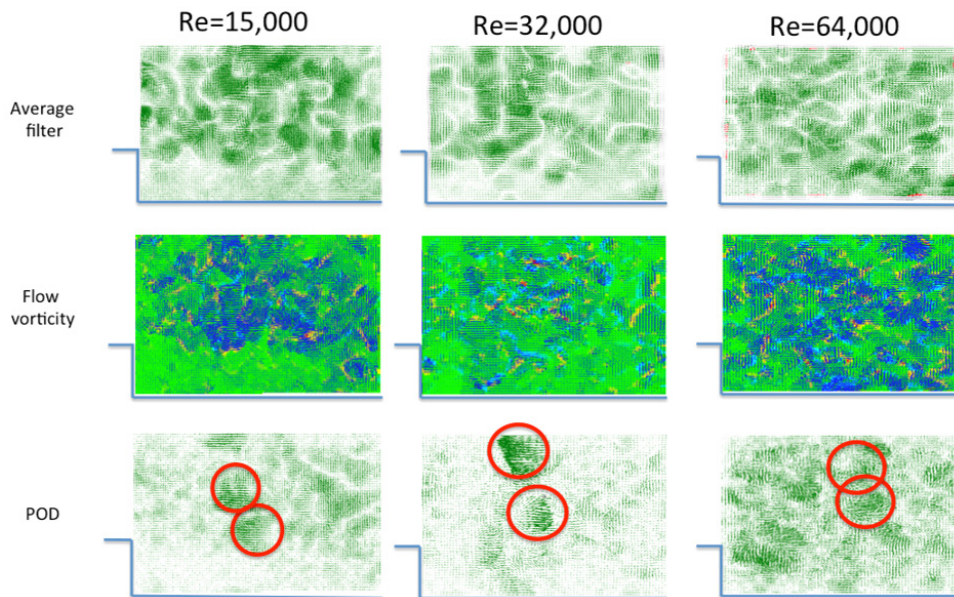
FIGURE 6
PIV Analysis for three different test conditions. H-PLIF at 283nm excitation was used to map flame front characteristics at the three different flow rates (Re=15000, Re=32000, Re=64000) at a rate of 10 kHz.
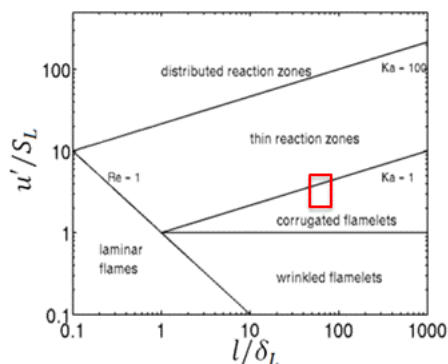

FIGURE 7
Borghi diagram with operating range indicated by red box.

E. Investigation of Piezoelectric Reactives as Tunable Energetics
Professor Sally Bane, Purdue University, STIR Award

The effort to realize advanced munitions through the use of high-performance and safe energetic materials has led to interest in nano-composite energetic materials. A particular class of energetic materials, nano-aluminum/fluoropolymer composites, are of interest due to their high densities and performance-enhancing capabilities in explosive, propellant, and pyrotechnic applications. In particular, the nano-aluminum (nAl)/fluoropolymer system has been demonstrated to exhibit susceptibility to ignition sensitization by means of charge application, potentially due to the piezoelectric properties of the fluoropolymer. However, the mechanism through which sensitization is possible was not evident. Therefore, the following objectives were proposed: (1) the development of synthesis procedures for nano-aluminum/fluoropolymer composites for the consistent and controlled production of samples for small-scale testing; and (2) the investigation of the sensitization of nAl/fluoropolymer composites by charge application, electrical poling, and inert doping and the subsequent combustion characteristics to identify the mechanisms responsible for sensitization susceptibility.

In FY16 several accomplishements were achieved. First, potential nAl/fluoropolymer systems were studied via Cheetah modeling to improve understanding of their ignition, combustion, and piezoelectric characteristics. Second, methods were developed for synthesizing nAl/fluoropolymer composite films for the consistent and controlled production of test samples. 80nm nano-Aluminum was used with a native alumina passivation shell resulting in 82wt% active aluminum. Two fluoropolymers were used: DyneonTM THV 221AZ, which is a terpolymer of tetrafluoroethylene (TFE), hexafluoropropylene (HFP), and vinylidene fluoride (VDF) with the empirical formula $C_{2.29}F_{4.33}H_{0.25}$, and Kynar® polyvinylidene fluoride (PVDF) with the empirical formula $C_2F_2H_2$. Both spin-casting and inkjet printing were investigated as deposition methods, although it should be noted that for larger samples, the polymers used are also suitable for casting. The resulting systems were thermodynamically characterized via differential scanning calorimetry (DSC) / thermogravimetric analysis (TGA) and surface morphology was characterized by SEM (see FIGURE 8).
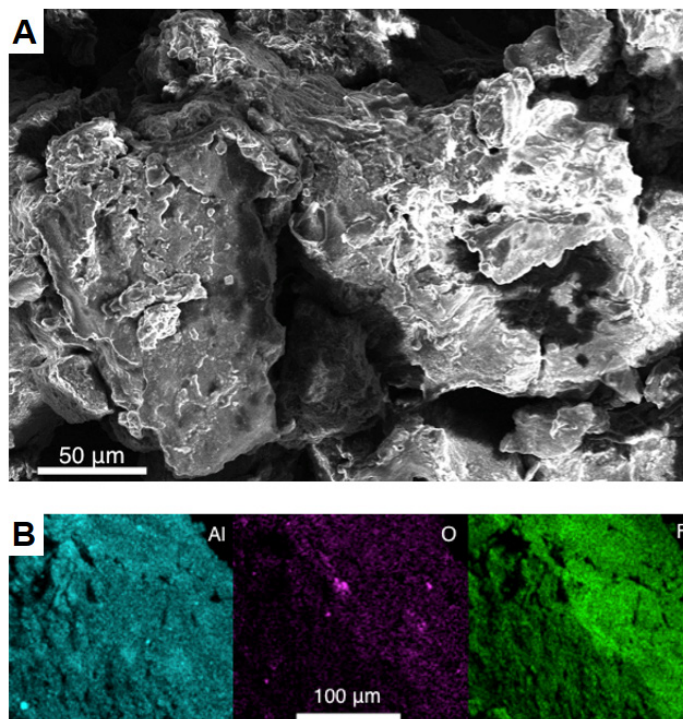

FIGURE 8

Characterization of the surface morphology of nAl/THV composite particles. (**A**) electron micrograp and (**B**) element map using energy dispersive spectroscopy.

Experiments were then conducted to investigate the sensitization of these composites by charge application, electrical poling, and inert doping. To confirm piezoelectricity, a variety of treated and untreated samples were placed between electrodes and subject to a constant controlled mechanical stress, and the voltage response was measured using an oscilloscope. The maximum of the voltage response for each system is shown in FIGURE 9. Piezoelectric behavior of the composites resulting from doping and electrical poling was demonstrated. Drop weight ignition experiments showed that the ignition sensitivity of electrically poled samples could be controlled using an electric field. Sheets of nAl/THV were placed between conductive copper electrodes, after which an external voltage of 1800V was applied and the samples were ignited from one end. The average burn rates were determined using high-speed videography and are shown in FIGURE 10. The results suggest that applying an external electrical field increases the burn rate of the samples substantially. It is known that increasing the net thermal conductivity of a sample, by means of a thermal conduit, increases the burn rate of composite samples. However, since copper electrodes surrounded both of the uncharged and charged samples, the burn rate enhancement cannot be attributed to the increase in thermal conductivity. Instead, it is suspected that the heat liberated from the reaction zone may have been transferred to unburned portions, lowering the dielectric strength. This resulting in premature ignition downstream of the burning surface due to dielectric breakdown. Hence, the application of a strong electric field, with a voltage near the ignition threshold of that of the

composite sample, appears to result in burn rate enhancement. Finally, nAl/THV composites were shown to be susceptible to photoflash ignition. These results demonstrate the potential for using these composites as tailored energetic materials and as additives for sensitivity control in other energetic systems.
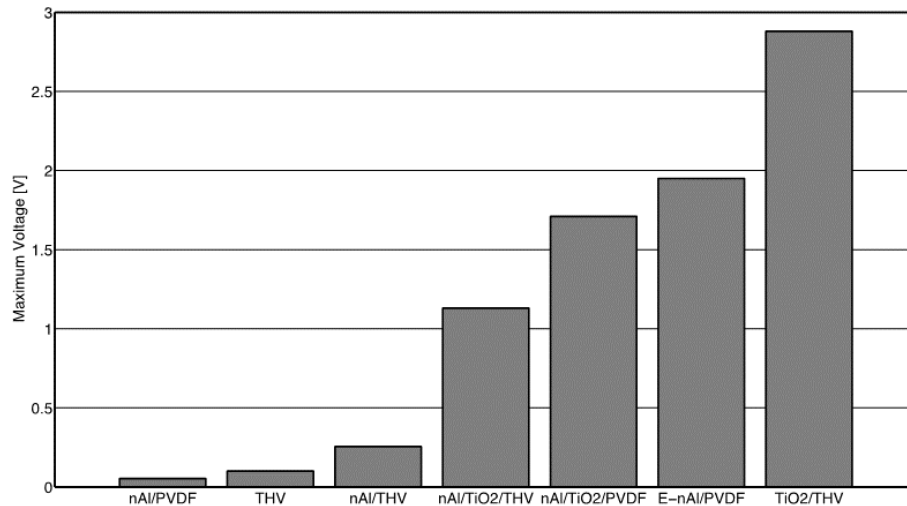

FIGURE 9

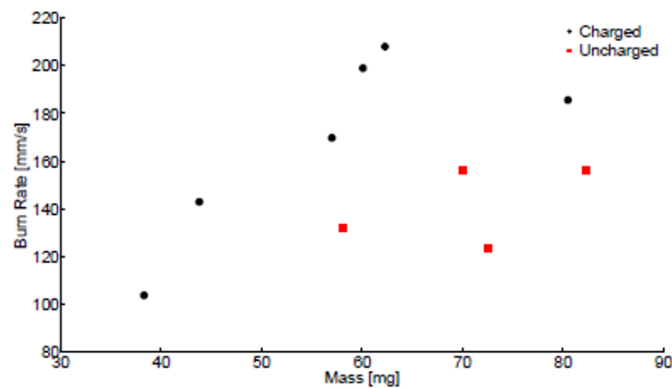Maximum voltage response due to mechanical stress for multiple nano-particle/fluoropolymer composite systems.

FIGURE 10

Burn rates of sheets of charged vs. uncharged in nAl/THV

F. Aerodynamic Control of Coupled Body-Wake Flow Instabilities on a Free-Moving Platform
Professor Ari Glezer, Georgia Institute of Technology, Single Investigator Award

Prior ARO supported research demonstrated that enhancement or suppression of reciprocal coupling of a stationary bluff body and its wake had a substantial impact on the evolution and stability of the wake and the resultant aerodynamic loads on the body. The currently supported effort extends these results by examining the unsteady flow physics associated with a body undergoing dynamic motions. In FY16, wind tunnel experiments were performed to characterize the uncontrolled and controlled behavior of a bluff body in near free-flight conditions. The model was supported by eight servo-controlled wires and was programmed to execute prescribed time-dependent yaw/pitch motions. Fluidic actuation was effected using an azimuthal array of four hybrid synthetic jet actuators equally distributed about the aft end of the body and led to partial, segmented attachment of the nominally azimuthally-separated shear layer. This control produced controlled wake asymmetries accompanied by variations of the aerodynamic loads. A specific goal of this effort was to demonstrate that this approach would be sufficiently robust to control the wake in combined canonical pitch and yaw motions designed to mimic the unstable response of an airborne platform (in the absence of roll). This was

accomplished using flow control strategies to either decouple the body from its near-wake dynamics or to amplify the unstable wake response to the motion. The flow evolution was characterized using time resolved aerodynamic load measurements and high-resolution stereo particle image velocimetry (PIV) measurements in the near-wake in a cross stream plane normal to the oncoming flow (and to the model's axis at rest) at one body diameter downstream of the model's aft end. Enhancement and suppression of motion-induced aerodynamic loads on the model were investigated at reduced frequencies of up to k = 0.26, ranging from a stationary model (k = 0), to quasi-steady (0 < k < 0.05) and unsteady (0.05 < k < 0.26) motions.

Two flow control strategies were demonstrated when the model was undergoing the combined pitch/yaw motions. The first strategy focused on decoupling the wake response from the model's motion, and was designed to render the wake's response invariant and equivalent to the wake of the nominally stationary model. The second strategy was designed to intensify the response of the wake to the prescribed motion of the body to mimic larger angular pitch/yaw deflection. These strategies were applied at reduced frequencies within the range 0.017 < k < 0.259 and yielded up to 75% reduction or 100% augmentation of the motion-induced side and lift forces without an increase in drag. Alternatively, the actuation could lead to variation of the motion-induced pitch and yaw moments resulting in 80% reduction or 40% augmentation, without affecting the roll moment.

These investigations demonstrated that the effects of the actuation on the model's near wake are comparable to the effects of its unstable pitch/yaw motions in the absence of actuation and therefore point to their potential for generating aerodynamic loads that can suppress or enhance the unstable aerodynamic loads to promote dynamic steering and stabilization, clearly demonstrated in the representative case shown in FIGURE 11 (Reynolds number based on diameter is 1.8×10^5). For a prescribed pitch/yaw motion (a,b), the uncontrolled baseline load coefficients (c: side force, d: lift force, e: yaw moment, f: pitch moment) are shown in blue, with force suppression control in green and force amplification control shown in red.
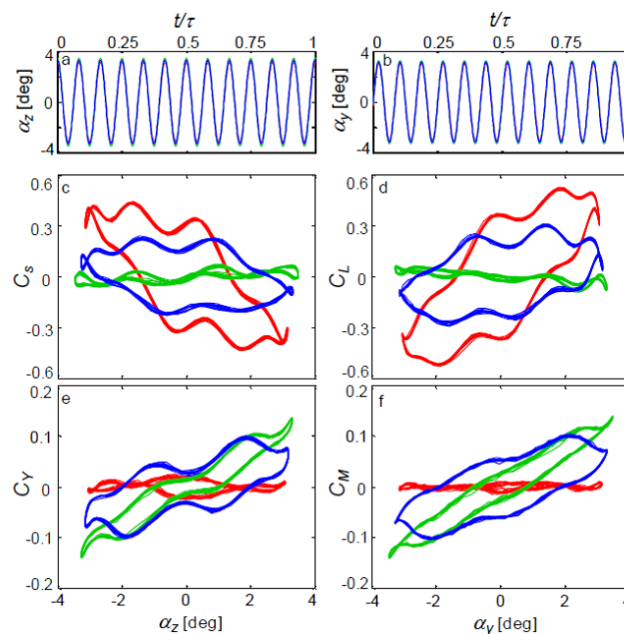

FIGURE 11

Angular motion (a,b) and variation in induced force (c,d), and moment (e,f) for *k*=0.207 without (blue) and with the flow control schemes for force suppression (green) and augmentation (red) at Re_D = 1.8×10^5.

G. Sedimentation, Orientation and Dispersal of Ramified Particles in a Turbulent Environment
Professor Donald Koch, Cornell University (lead) and Professor Greg Voth, Wesleyan University, Single Investigator Award

This research seeks to develop models of the dynamics of anisotropic particles in turbulent flows. The particles possess a ramified structure consisting of interconnected rods of varying lengths, diameters and relative orientations, much like the six-pointed jack from the children's game. The research effort combines

development of theoretical models and numerical simulations (Professor Koch) along with experiments in a turbulent flow facility (Professor Voth). The main thrust of this work is to develop a descriptive and predictive understanding of the way in which the fluid inertia associated with a settling non-spherical particle competes with turbulent velocity fluctuations to determine the settling behavior, orientation and dispersion of particles settling in a homogeneous isotropic turbulent flow. The orientational and translational dynamics are primarily goverened by the particles' size, symmetry, and settling velocity. When a particle is smaller than the Kolmogorov length scale (η), the particle experiences turbulence as a temporally fluctuating local linear velocity field. Conversely, when the particle is much larger than η, the local flow field now couples nonlinearly with the particle, which is most responsive to eddies whose size is comparable with the dominant particle length scale. Additionally, when the particle settling velocity is much smaller than these eddies the particle translates primarily due to the motion of the fluid. When the particle settles much faster, the particle samples a nearly frozen turbulent velocity along its trajectory.

In FY16, a vertical water tunnel facility was constructed and validated for the measurement of 3D particle orientation and translation in a turbulent field (see FIGURE 12). Theories predicting the orientation distribution of small fibers (relative to η) settling in a turbulent flow have also been developed. Finally, asymmetric and branched particle shapes have been examined and found to allow particles to orient and settle obliquely even in the absence of turbulence, permitting horizontal dispersion of particles in environments characterized by a broad range of turbulent behavior. Above a critical Reynolds number (based on sedimentation velocity), the particle no longer falls with the major axis aligned with gravity, but instead exhibits a bifurcation, where the particle assumes an oblique angle based on the balance between torques induced by inertial and gravitational forces. Continuing efforts will explore the parameter space of particle shape, asymmetry, size, sedimentation number and turbulent intensity. Experiments, numerical simulations and theoretical model development will occur synergistically, with each effort informing and validating the others.
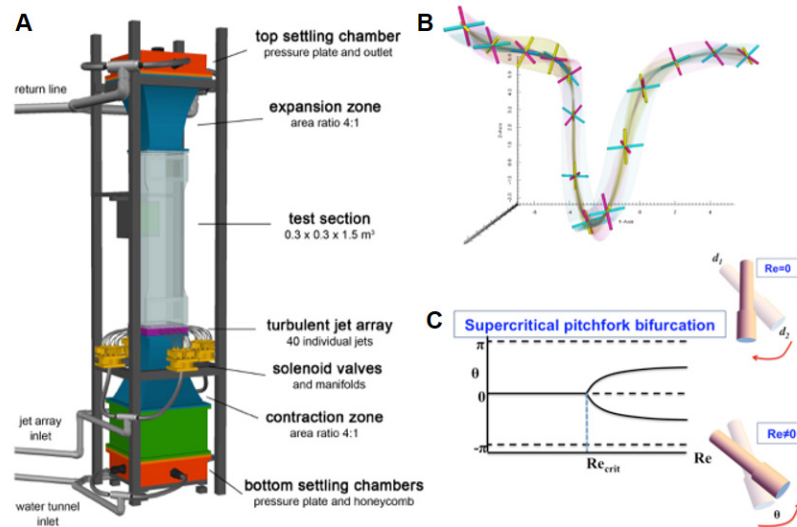

FIGURE 12

Vertical water tunnel facility. The facility was constructed and validated for the measurement of 3D particle orientation and translation in a turbulent field. (**A**) Vertical turbulent flow facility schematic; (**B**) ramified particle trajectory in turbulent flow from 3D photogrammetry experiment; (**C**) bifurcation behavior of asymmetric particle in quiescent flow.

IV.   TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Augmented Finite Element Method for High-Fidelity Analysis of Structure Composites
Investigator: Professor Qingda Yang, University of Miami - Coral Gables, Single Investigator Award
Recipients: ARL-WMRD and Boeing Corp.

The objective of the project is development of an efficient and accurate multiscale computational methodology for rapid virtual testing of composites with complex microstructures. The research goals include: (i) the development of new 2D and 3D A-FEM elements that can explicitly account for statistical material heterogeneity and can reliably predict progressive damage initiation, propagation and multi-crack interaction; and (ii) to apply the new method to study composites of interest to the Army, coupled with 3D μCT-based precision experiments, to understand key physical phenomena of crack formation and growth, and to quantify their direct effects on structural integrity under general loads. To achieve these goals, the following tasks have been performed: development of an efficient and robust Augmented-FEM-based simulation platform for 2D and 3D heterogeneous materials so that microscopic damage evolution and resulting structural performance degradation can be predicted concurrently; development of geometric and material models that realistically reflect the statistics of reinforcement architecture and random distribution of material heterogeneity; validation of prediction fidelity via micro-computer-tomography (μCT) at microscopic scale and surface digital image correlation technique at a structural scale. The code developed in the course of this project has transitioned to scientists at ARL-WMRD and Boeing Corp. for potential applications for fatigue cohesive zone crack growth model.

B. Surface Chemistry and Combustion Behavior of Hypergolic Solid Fuels
Investigator: Professor Steven Son, Purdue University, Single Investigator Award
Recipient: AMRDEC

The objective of this research is to develop a fundamental understanding of the controlling mechanisms of heterogeneous reactions of gaseous/liquid oxidizer and solid fuel combinations through the study of fuel/oxidizer combustion in opposed burners and tube combustors as well as the development of several novel experimental techniques. This work led to the investigation of novel ammonia borane based hypergolic hybrid propellants, for which ignition delay time data has transitioned to AMRDEC for evaluation. Additionally, formulation information for novel binders compatible with ammonia borane have been provided to AMRDEC for their use in development of propellants. This was provided along with information on modification of the procedure by which the compatibility testing itself was completed.

C. Highly-Successful Empirical Theory for Mobility in Dry Granular Environments Explained
Investigator: Professor Ken Kamrin, Massachusetts Institute of Technology, Single Investigator Award
Recipients: Tank and Automotive Research, Development and Engineering Center (TARDEC)

The objective of the research is to determine a theoretical underpinning for a highly successful but empirical Resistive Force Theory (RFT) model of granular intrusion and locomotion. To date, the dynamics of granular media has been without precise constitutive relations. This question has nagged scientists for centuries, going back to Coulomb, due to the fact that granular behavior is simultaneously nonlinear, history-dependent, rate-sensitive, and nonlocal. Army supported work on mobility of robots using RFT revealed a simple explanation for intrusion forces on a generally-shaped object in spite of all the complications that characterize granular mechanics. Until this year, there was no theoretical explanation for this observation. The PI, after conducting many continuum simulations, was able to identify that perfectly-plastic frictional rheology generates all the RFT hypotheses and replicates existing sets of experimental data used as inputs for RFT. Because frictional plasticity

depends on so few material parameters, a dimensional analysis was then able to explain why RFT emerges in dry grains, whereas in other materials that "should" be simpler (e.g. linear viscous fluids) the RFT idea does not work as well. Pushing forward, using the same analytical technique, the PI predicted that a family of pasty materials obeying a simple constant yield-stress flow rule should also possess a strong RFT. This prediction was then directly confirmed in finite-element tests, revealing that the analytical approach discovered by the PI may function like a diagnostic tool for discerning whether a given material obeys RFT.

The results of this research transitioned to TARDEC, which then opened a new area of research based on the analytical approach to identify scaling relations that will enable predictive modeling of impulsive shear and intrusion into granular media for robotics and large ground vehicles spanning the millimeter to the meter scale.

D. Passive Bio-Inspired Separation Control Mechanism Derived from Shark Skin
Investigator: Professor Amy Lang, University of Alabama - Tuscaloosa, Single Investigator Award
Recipients: Boeing Corp.

The goal of this research project is to investigate whether the bristling of shark scales represents a passive mechanism by which flow separation is controlled. Flow separation is often preceded by flow reversal in the bottom few percent of the boundary layer thickness. The working hypothesis of this effort is that the bristling of shark scales is induced by this flow reversal and serves to disrupt the incipient separation event. Two mechanisms are proposed for this disruption (i) the bristled scales locally impede further flow reversal and (ii) the cavities formed between the scales induce mixing of high-momentum fluid towards the wall. An experimental campaign is underway to characterize the behavior of real shortfin mako skin in a water channel. Time-resolved particle image velocimetry will be used to analyze the behavior of the fluid behavior in the boundary layer and describe the extent of separation control and the relevant mechanism.

The project has potential to not only describe an interesting biological boundary layer control mechanism, but also to inform the design of an engineered material that will perform the same task for wall-bounded flows. Boundary layer control has been a long-sought engineering objective, but usually fails to make the transition to full-scale engineering platforms due to the size, weight or power requirements of the actuation scheme. If the observed phenomena is able to be scaled appropriately, future DoD vehicle and weapons delivery platforms may achieve significant gains in performance by passively inhibiting separation. In pursuit of this objective, The Boeing Company has invested research funding alongside the ARL-ARO investment to explore the issues relevant to conducting wind tunnel experiments and to accelerate the development of an engineered "shark skin" analog. Advances in fundamental understanding of the mechanisms coupled with the technology development efforts to mimic the effect may provide a new capability in the near future.

Many of these results transitioned to Boeing Corp, which is now funding Professor Lang's laboratory to test actual shark skin in an air environment to identify if the scale bristling occurs under non-aqueous conditions. Boeing funding is also supporting the development of an engineered (3D-printed) shark skin analog for use on aerodynamic vehicles. This work will explore issues associated with scale shape, roughness, hinging, and size to determine the effectiveness of the engineered skin to passively prevent boundary layer separation.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Modeling Rate Dependent Dissipation in Granular Solids via Continuum Thermodynamics
Professor Giuseppe Buscarnera, Northwestern University, STIR Award

The objective of this research is to formulate multi-scale models able to express the dissipative capacity of heterogeneous granular solids in light of their inherent particulate nature. For this purpose, it is planned to bridge continuum thermodynamic laws accounting for different forms of dissipation (e.g., friction, plastic compaction, grain crushing) to particle-scale models of elastic energy storage, fracture and rate-dependent crack growth. The goal is to provide simulation tools transferable to large-scale computations for dynamic analyses, as well as to (i) explain the significance of grain scale attributes (e.g., size, shape, degree of polydispersity, mineral composition, patterns of fragmentation) and (ii) use this new understanding to design granular barriers with tunable dissipative properties.

The research approach includes: (1) Formulation of energy scaling hypotheses linking the energy released by a granular matrix undergoing distributed comminution to the energy released by fractured particles. (2) Analytical derivation of the energy stored in particles at the onset of fracture for three contact laws (linear, Hertzian and conical contacts) and two fracture models (central split and contact fracture). (3) Microscopic characterization of two granular solids (spherical glass beads and angular quartz sand; with grading ranging from fine (i.e., grain size of 150 μm) to coarse particles (i.e., grain size of about 1mm). (4) Conduction of diametrical compression tests on single particles via a miniature compression device. (5) Conduction of one-dimensional compression tests on packed samples by means of a high-capacity loading frame and dedicated stainless steel compression cells. (6) Calibration of the continuum thermodynamic model based on the evidences from the testing program and simulation of the deformation response of granular assemblies.

Granular media are among the most manipulated materials in industry. It is thus arguable that an improved understanding of their complex behavior will have a profound impact on technology. In FY17, this exploratory project will set a vision for the extension of the multi-scale continuum modeling of comminution to a wide range of stress states and multi-physical interactions (e.g., adsorption/desorption of fluids or changes in temperature during impact). This research has thus the potential to impact numerous problems based on the physics of granular matter, such as remote exploration, penetration monitoring at inaccessible locations, design of granular barriers, and earth machine interaction, thus fostering a line of research that is crucial for both civilian and military applications.

B. Nonlinear Dynamics and Distributed Control for Soft Robot Locomotion
Professor Derek Paley, University of Maryland; Professor Carmel Majidi, Carnegie Mellon University (CMU); Professor Oliver O'Reilly, University of California – Berkeley; Single Investigator Award

The objective of this research is to construct a mathematical framework for real-time control of a soft robot system through dynamical modeling and sensor feedback. The dynamics and control framework will be validated on an experimental testbed to include soft, limbed robots powered by dielectric-elastomer actuators and shape-memory alloy. In contrast to their conventional rigid counterparts, soft machines and robots are elastically deformable bodies capable of extreme changes in shape and functionality. Progress in the nascent field of soft robotics depends on the ability to rapidly and faithfully model the dynamical state of a soft robot and incorporate this model into a feedback control for real-time path planning and locomotion. This research program has three tasks: (1) iterative construction of a hierarchical modeling framework to describe legged locomotion using nonlinear dynamics and continuum mechanics in a manner conducive to control (lead: Oliver O'Reilly, University of California – Berkeley); (2) empirical and theoretical study of tribological interactions for ground contact with a soft robot limb (lead: Carmel Majidi, Carnegie Mellon University); and (3) design and

implementation of a distributed controller for legged locomotion using sensor feedback (lead: Derek Paley, University of Maryland – College Park). In FY16, the following plans for each respective task are as follows: (1) for modeling, the O'Reilly laboratory will develop a hierarchy of models for the locomotion of a soft limbed robot. These models will include discrete models where the robot is modeled using a system of particles and rigid bodies, finite element models, and rod and string based models. Discretization of the latter models will feature models of the first two types. Concomitant with the model development, parallel efforts in the quantification of the parameters needed for the models and validation of the resulting models will be performed.; (2) for empirical interactions, Professor Majidi will focus on developing a soft robot testbed with novel elastomer shape-memory-alloys as intrinsic "artificial muscle" actuators for powering locomotion as well as flexible electronics for on-board power; and (3) for distributed control, Professor Paley will approach soft-bodied locomotion in biology as a circular network of connected nodes. Professor Paley will study synchronization and consensus of coupled node oscillators through a damping and spring connection. When the damping coefficient is smaller than the damping attenuation, the system may not achieve consensus before the oscillations die out. Parametric analysis will be performed and tested in the robotic testbed being developed at CMU.

C. Spatially and Temporally Resolved Imaging of Primary Breakup in High-Pressure Fuel Sprays
Professor Caroline Genzale, Georgia Institute of Technology, Young Investigator Award

The objective of this effort is challenge long-standing empirical views on the mechanisms of atomization in high-pressure fuel sprays via microscopic imaging of high Reynolds number liquid jets. The work specifically seeks to address the role of aerodynamic shear and liquid turbulence on interfacial instabilities and subsequent atomization outcomes, resolving discrepancies in the in the literature which have attributed high-pressure liquid jet atomization to both physical mechanisms. To enable adequate temporal and spatial resolution for study of the problem, a new ultrahigh- resolution transient imaging technique, termed "spectral microscopy," is proposed for development. This novel measurement technique employs a ns-scale pulsed multi-color LED illumination system coupled with a high-resolution 16 MP color CCD camera and microscopic lens. Sequenced pulsing of the colored LEDs, with spectrally isolated detection of each imaging pulse at the RGB sensor, will enable the capture of three-image sequences of the liquid interface in high-pressure fuel sprays at O[μm] spatial and O[ns] temporal resolution. An equivalent imaging speed of 50M fps will be achieved, representing a 50x speed up over current high-speed cameras, with a concomitant 16-20x increase in field-of-view. It is anticipated that in FY17, the novel measurement technique will be completed and demonstrated, allowing direct investigation into the role of the aerodynamic shear on spray breakup.

D. Asymmetric Vortex Control on Slender Bodies at High Angles of Incidence
Professor Rajan Kumar, Florida A&M University, Single Investigator Award

The objective of this research is to improve understanding of the source and nature of vortex asymmetry on slender cones at high angles of incidence. Vortex asymmetry on conical axisymmetric forebodies leads to undesirable side forces and yawing moments that can affect the control characteristics of such bodies and limit the performance and maneuverability. As can be seen in FIGURE 13, for a slender cone at 40° incidence angle, as the cone is rolled about its longitudinal axis, the vortex development switches sides, leading to a sign change in the resultant side force (shown in the line plot). The mechanisms for the development of this asymmetry are not well understood, but may be due to the presence of random micro-imperfections in the apex region, which provides perturbations to the developing boundary layer. The process by which the flow amplifies these disturbances, which ultimately leads to the symmetry breaking, is poorly characterized. This study is performing a systematic experimental, computational and theoretical investigation to determine the importance of these imperfections and identify the relevant mechanisms of instability growth. As these mechanisms are discovered and explained, a physics-based flow control system to mitigate induced side forces and yawing moments will be developed.
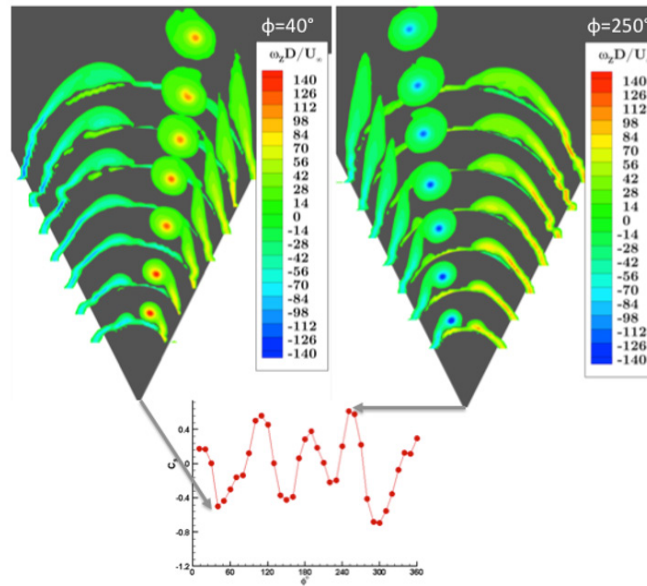
FIGURE 13

Vortex formation on a slender cone at 40° incidence angle for two roll angles, φ = 40°and φ = 250. Vortex asymmetry is clearly demonstrated in both cases (contour colors are non-dimensionalized axial vorticity). The resulting side force (line plot) clearly demonstrates the change in sign of the side force coefficient due to the asymmetry.

In FY16, a set of baseline measurements were performed on a pair of 12° semi-apex angle cones. The role of the micro-imperfections was examined, via force and flowfield diagnostics. The experimental data was used to validate a computational effort, which allowed a stability analysis to be performed. In FY17, it is anticipated that the effect of Mach and Reynolds number variation on vortex asymmetry development will be characterized experimentally, along with measurement of the growth rate and coupling dynamics of perturbations in the boundary layer. Numerically, controlled perturbation s will be introduced on the surface of the cone, which will allow the identification of the length and time scales associated with asymmetric vortex development and interaction. Some effort will be undertaken to begin exploring potential control methodologies that may be effective in restoring symmetry by preventing the growth of boundary layer instabilities.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Ralph Anthenien
Division Chief
Program Manager, Propulsion and Energetics

Dr. Samuel Stanton
Program Manager, Complex Dynamics and Systems

Dr. Asher Rubinstein
Program Manager, Solid Mechanics

Dr. Matthew Munson
Program Manager, Fluid Dynamics

B. Directorate Scientists

Dr. David M. Stepp
Director, Engineering Sciences Directorate

Dr. April Brown (IPA)
Research Scientist

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. LaToya Guidry
Administrative Specialist

CHAPTER 10: NETWORK SCIENCES DIVISION

I.   OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2016* is to provide information on the programs and basic research supported by ARO in fiscal year 2016 (FY16), and ARO's mission to create basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Network Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY16.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Network Sciences Division supports research to discover mathematical principles to describe, control, and to reason across the emergent properties of all types of networks (*e.g.*, organic, social, electronic) that abound all around us. The unprecedented growth of the internet, the tremendous increase in the knowledge of Systems Biology, and the availability of video from US military operations have all led to a deluge of data. The goal of the Network Sciences Division is to identify and support research that will help create new mathematical principles and laws that hold true across networks of various kinds, and use them to create algorithms and autonomous systems that can be used to reason across data generated from disparate sources, be they from sensor networks, wireless networks, or adversarial human networks, with the resulting information used for prediction and control. Given that network science is a nascent field of study, the Network Sciences Division also supports basic research on metrics that are required to validate theories, principals and algorithms that are proposed.

2. Potential Applications. Research managed through the Network Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO through network science research may provide new and revolutionary tools for situational awareness for the Solider and new regimes for command, control and communication for the Army. Furthermore, work supported by ARO through the Network Sciences Division could lead to autonomous systems that work hand-in-glove with the Soldier.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Network Sciences Division frequently coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In particular, the Division's portfolio is coordinated with the ARL Information Science, Computing Science, and Human Sciences Campaigns by both influencing the development of Campaign strategies, and by being cognizant of the Campaigns' needs.   In addition, the Division frequently coordinates with other ARO Divisions to co-fund research, identify multi-disciplinary research topics, and to evaluate the effectiveness of research approaches. For example, interactions with the ARO Computing Sciences Division include promoting research to investigate game-theoretic techniques that could lead to better cyber situational awareness and to address concerns about performance and resilience to cyber attacks in ad-hoc dynamic wireless networks in a uniform fashion. The Network Sciences Division also coordinates its research portfolio with the Mathematics Division to pursue studies of game theory that address bounded rationality and human social characteristics in a fundamental way. The Network Sciences Division coordinates with Life Sciences on studies at the neuronal level to understand human factors in how decisions are made under stress. Lastly, the Division's Program Areas interface with the Mechanical Sciences Division to understand the interplay

between learning and manipulation and locomotion in robotic systems. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

The Network Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY16, the Division managed research within these four Program Areas: (i) Multi-agent Network Control, (ii) Decision and Neuro Sciences, (iii) Communications and Human Networks, and (iv) Intelligent Networks. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Multi-agent Network Control. The Multi-Agent Network Control program has a long, successful history in providing new scientific results and leadership concerning the mathematical foundations for the robust control of complex real-time physical and information-based systems. The program was among the first in the DoD to recognize the need and potential for mathematical control theory to be pushed toward the heterogeneous multi-agent and (semi)autonomous domain, leading to a strong record of success in the distributed control of autonomous agents as well as the control of micro-biological systems. Concurrent with these developments, the scientific community became keenly aware of the role of interconnections, and dynamics over these interconnections, on the ensuing behavior of finite (oftentimes large) numbers of agents (in the abstract sense). This subsequently led to the burgeoning discipline of "network science" for which principles were sought and discovered and often found a broad range of applications spanning the physical, biological, and social sciences. While discovery and understanding of complex systems in nature, economics, and society are of profound value and impact, our ability to exploit this knowledge to engineer the controllability, fragility, propensity for self-organization, and/or robustness of interdependent dynamical systems will inevitably demonstrate true mastery. Creating the relevant theory to adapt and control science in this regard has emerged as a focal point for future programmatic efforts. An overarching, principled framework has yet to be established and requires not only control theory, but also dynamical systems, information processing, and phenomenological physics. Thus, the mission of the Multi-Agent Network Control program is to establish the physical, mathematical, and information processing foundations for the control of complex networks. In view of complementary ARO Network Science Division efforts spanning intelligent, communication, and sociological networks, the main focus of the program will primarily involve physical and biological networks but in an abstract framework potentially extensible to network models relevant to all division portfolios. This Program Area is divided into three research thrusts: (i) Control and Dynamical Systems Theory, (ii) Information Structure, Causality, and Dynamics, and (iii) Physics in the Control of Complex Networks. These thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal.

2. Social and Cognitive Networks. The goal of the Social and Cognitive Networks program is to develop measures, theories, and models that capture cognitive and behavioral processes that lead to emergent phenomena in teams, organizations, and populations. Social networks allow collective actions in which groups of people can communicate, collaborate, organize, mobilize, or attack. Social influence processes determine how ideological groups form and dissolve, information and beliefs spread and interact, and how populations reach consensus or contested states. Research supported in this program includes both methodological aspects of modeling human networks and substantive work to further our understanding social and emergent phenomena. Methodological projects focus on statistical network analysis, computational models and dynamic simulations that address issues such as scalability, multilayers, and data accuracy (i.e., investigating effects of measurement error on metrics and inferences due to missing, inaccurate or hidden network data). Substantive research focuses on cognitive and psychological factors that drive social phenomena, including development of new metrics, constructs and mechanisms involved with complex activities such as information transfer/exchange and collective decision-making. This program invests in innovative solutions that blend theories and methods from the social sciences with rigorous computational methods from computer science and mathematical modeling. The changing nature of DoD's doctrines and missions have greatly increased the need for models that capture the cognitive, organizational and cultural factors that drive activities of groups, teams and populations. The program seeks to advance our understanding of the human dimension and provide critical insights about team coordination and

problem solving, social diffusion and propagation, and develop tools that enable inference and modeling of complex social phenomena.

3. Communications and Human Networks. The goal of this Program Area is to better understand the fundamental scientific and mathematical underpinnings of wireless communications and human networking, their similarities, and the interactions between these two networks. This Program Area is divided into two research Thrusts: (i) Wireless Communications Networks and (ii) Human Networks. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research to pursue the program's long-term goal. The Wireless Communications Networks Thrust supports research to discover the fundamental network science principles as they apply to the wireless multi-hop communications systems, while the Human Networks Thrust identifies and supports research to better understand social network structures from heterogeneous data, the structures effect on decision making, and the interaction of communications and human networks. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include wireless tactical communications, improved command decision making, and determining the structure of adversarial human networks.

4. Intelligent Networks. The goal of this Program Area is to develop and investigate realizable (i.e., computable) mathematical theories, with attendant analysis of computational complexity, to capture common human activity exhibiting aspects of human intelligence. These studies may provide the foundation for helping augment human decision makers (both commanders and Soldiers) with enhanced-embedded battlefield intelligence that will provide them with the necessary situational awareness, reconnaissance, and decision making tools to decisively defeat any future adversarial threats. This Program Area is divided into two research Thrusts: (i) Integrated Intelligence and (ii) Adversarial Reasoning. These thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long term goal. The Integrated Intelligence Thrust supports research to discover the mathematical structuring principles that allows integration of the sub-components of intelligent behavior (such as vision, knowledge representation, reasoning, and planning) in a synergistic fashion, while the Adversarial Reasoning Thrust area brings together elements of Game Theory, knowledge representation and social sciences to reason about groups/societies in a robust manner. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include robotic unmanned ground and air vehicles, reasoning tools for wild life management, and decision making tools in the context of command, control, communications, computers, intelligence, surveillance and reconnaissance (C4ISR).

C. Research Investment

The total funds managed by the ARO Network Sciences Division for FY16 were $47.0 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $7.1 million and $2.0 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $5.2 million to projects managed by the Division. The Division also managed $28.0 million of Defense Advanced Research Projects Agency (DARPA) programs, and $1.5 million was provided from other Army laboratories. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.7 million for contracts. In addition, $3.4 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $1.9 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY16 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY16 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY16, the Division awarded 19 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Emmanuel Abbe, Princeton University; *Information-geometric Embeddings for Feature Extraction in Networks*

- Professor Nitin Agarwal, University of Arkansas at Little Rock; *Towards Predictive Modeling Deviant Cyber Flash Mobs: A Socio-Informatics Driven Hypergraph Framework*

- Professor Javad Ghaderi, Columbia University; *Distributed High Performance Algorithms for Mobile Ad Hoc Networks*

- Professor Syed Jafar, University of California - Irvine; *Optimal Use of Multiple Antennas in Tactical Interference Networks - MIMO, IA and Beyond*

- Professor Kristina Lerman, University of Southern California; *Measuring and Mitigating the Impact of Network Bias on Computation in Graphs*

- Professor Kyle Lewis, University of California - Santa Barbara; *Tasks and Transitions: An Investigation of Transactive Memory Systems in Teams Performing Multi-Task Activities*

- Professor Chjan Lim, Rensselaer Polytechnic Institute; *Mathematical and Computational Studies of Realistic Aspects of Social Contagions and Cascading Instabilities on Networks*

- Professor Michael Mahoney, International Computer Science Institute; *Local Algorithms for Large Informatics Graphs*

- Professor Brandon Minnery, Wright State University; *Maximizing the Collective Intelligence of a Network Using Novel Measures of Socio-Cognitive Diversity*

- Professor Nicholas Ouellette, Stanford University; *Macroscopic Properties and Microscopic Interactions in Insect Swarms*

- Professor Filippo Radicchi, Indiana University at Bloomington; *Structural and Dynamical Transitions in Networks of Networks*

- Professor Anna Rumshisky, University of Massachusetts - Lowell; *Detecting Civil Conflict and Information Biases in Polarized Environments in Social Media*

- Professor Michelle Shumate, Northwestern University; *Collective Impact and Common Goals: Planned vs. Emergent Networks as Tools for Leveraging Community Outcomes*
- Professor Kelland Thomas, Stevens Institute of Technology; *Musical Improvising Collaborative Agent*
- Professor Hanghang Tong, Arizona State University; *Towards Optimal Teams in Composite Networks*
- Professor Panagiotis Tsiotras, Georgia Tech; *Statistical Mechanics for Learning Algorithmic-Based Controllers: The Role or Physics in New Computational Models for Real-Time Control*
- Professor Yevgeniy Vorobeychik, Vanderbilt University; *Designing Resilient Data Processing Systems for Adversarial Environments*
- Professor Jamil Zaki, Stanford University; *Attitude Convergence in Small Networks*
- Professor Junshan Zhang, Arizona State University; *Integrated Cognitive Mobile and Social Networking*

2. Short Term Innovative Research (STIR) Program. In FY16, the Division awarded six new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Animashree Anandkumar, University of California - Irvine; *Tensor Methods for Large-scale Learning*
- Professor Joseph Halpern, Cornell University; *Limited Learning, Rational Inattention, and Unawareness in Games and Decision Problems*
- Professor Brian P. Mann, Duke University; *Dynamics of Networks with Delays*
- Professor Ravi Mazumdar, University of Waterloo; *Causality and Information Dynamics in Networked Systems with Many Agents*
- Professor Tuomas Sandholm, Carnegie Mellon University; *Initial Computational Research on Steering T Cell Differentiation*
- Professor Sanjay Shakkottai, University of Texas at Austin; *Optimizing Human Input in Social Network Analysis*

3. Young Investigator Program (YIP).

No new starts were initiated in FY16.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY16 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Network Frontier Workshop 2015*; Evanston, IL; 6-7 December 2016
- *Workshop on Adaptive Defense in the Cyber-Security Domain*; Los Angeles, CA; 3-4 February 2016
- *International Network for Social Network Analysis Sunbelt Conference*; Newport Beach, CA; 5-10 April 2016
- *Workshop on Software Defined Networking*; New Haven, CT; 5-6 May 2016
- *Workshop on Opinion Dynamics*; Austin, TX; 13-14 June 2016
- *MIT Institute for Data, Systems, and Society Launch Event*; Cambridge, MA; 22-23 September 2016

5. Special Programs. In FY16, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded six new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant

portion of the basic research programs managed by the Network Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Scalable, Stochastic and Spatiotemporal Game Theory for Adversarial Behavior. This MURI began in FY11 and was awarded to a team led by Professor Milind Tambe of the University of Southern California, with participation from researchers at UCLA, Duke University, Stanford University, UC Irvine and California State University at Northridge. The objective of this MURI is the development of game theory formalisms that account for bounded rationality, scalability of solutions, real-world adversaries, and socio-temporal issues. The technical approach to be followed by the team will involve a mix of behavioral experiments and development of theoretical formalisms to characterize individual human behavior and that of adversarial groups; it is expected that psychological theories such as prospect theory and stochastic theories for coalitional games will play equal part in the technical development. The results of this MURI may have significant impact on diverse applications of the Army such as the monitoring of contracts while building nations or societies.

2. Evolution of Cultural Norms and Dynamics of Socio-Political Change. This MURI began in FY12 and was awarded to a team led by Professor Ali Jadbabaie of the University of Pennsylvania, with participation from researchers at MIT, Stanford, Cornell, and Georgia Tech. The objective of this MURI is to find synergy in methods and models from work in social sciences, engineering, network sciences, and mathematics to develop new techniques and mathematical models that would explain societal events not *posterior* but as they are happening, based on detailed analytical models of social systems. The team hopes to use a unified yet interdisciplinary lens that goes beyond social and political sciences, and adequately covers the full spectrum from rigorous math-based theory and modeling to large scale data extraction and analyses and from multi-agent simulation to controlled lab experiments and field surveys. The results of the MURI may have significant impact on the Army and DoD to understand cataclysmic changes, such as the Arab Spring, as they are about to happen.

3. Control of Complex Networks. This MURI began in FY13 and was awarded to a team led by Professor Raissa D'Souza of the University of California at Davis. The goal of this MURI project is to develop rigorous principles to predict and control behaviors of systems made of interdependent networks. This will be accomplished through an interdisciplinary approach synthesizing mathematical theories from statistical physics, control theory, nonlinear dynamics, game theory, information theory, system reliability theory, and operations research. The results will be informed and validated by empirical studies of real-world systems from nanoscale mechanical oscillators, to collections of interdependent critical infrastructure systems, to data on coalitions and conflict in primate societies, to longitudinal data on the evolution of political networks of nation states and task-oriented social networks in open source software. The focus is to develop new approaches that exploit network interdependence for network control, and this diversity of empirical testbeds is central to developing robust theoretical principles and widely applicable methods.

It is expected that this MURI will lead to (i) network interventions that prevent cascades of failure in critical infrastructures, (ii) novel control schemes relying on control actions and local interventions, (iii) rigorous principles for multi-modal recovery of heterogeneous systems, (iv) shaping human social response via designed incentives that align human behavior with the capabilities of technological networks, (v) design of networks of nonlinear nanoelectromechanical oscillators that exploit coupling and nonlinearity to create coherent motion, (vi) new mathematical structures for representing and analyzing networks-of-networks, especially with respect to control theory, and (vii) fundamental bounds on controllability of interdependent networks and rigorous techniques to identify which network layers are easiest to steer.

The anticipated impact on DoD Capabilities is broadly applicable to controlling a disparate collection of autonomous agents interacting through numerous networks in noisy, dynamic environments with a myriad of time-scales and length-scales. Results can be applied to security (and restoration) of critical infrastructures, supply chains, political alliance dynamics (including upheavals such as Arab Spring), conflict, risk, social dynamics, and collective action. It is also reasonable to expect that there will be new levels of nanoscale functionality in the NEMs device developed, enabling new technologies and devices.

4. Network Science of Teams. This MURI began in FY15 and was awarded to Professor Ambuj Singh of the University of California at Santa Barbara, with participation from researchers at University of Southern California, University of Illinois at Urbana-Champaign, Northwestern University, and MIT. These seven faculty provide an excellent balance of multidisciplinary scholars from sociology, cognitive and social psychology, health and behavioral sciences, computer science, statistics, controls and dynamical systems, and network

science. This MURI will advance the development of the Network Science of Teams by creating quantitative, network-based models of adaptive team behavior. This research will produce methods to optimize team performance under different contexts and resource constraints. The three thrusts of this research effort include (i) teams as networks of interacting entities, (ii) analysis and models of dynamic team behavior over task sequences, and (iii) the network science of teams-of-teams or multi-team systems. The overarching objectives of this research are to build quantifiable informative models of team behavior as dynamical systems interacting over multiple networks, to develop rigorous models that relate interaction patterns and network evolution to task performance, to break new ground in the learning of optimal design of teams for complex tasks, and to advance social science theories of team performance. This MURI will have a significant impact for the Army and DoD with respect to how it conducts its work in teams in that results from this research may help the Army and joint forces assemble more effective teams and teams of teams, and provide guidance on task sequencing to support their highest goals.

5. Multi-modal Analytics to Understand Latent Communication. This MURI began in FY16 and was awarded to a team led by Professor V. S. Subrahmanian of the University of Maryland. The goal of this MURI is two fold: (i) develop social science theories to understand latent communication among a small group of adversaries engaged in an effort to deceive, and (ii) develop multi-media analytics tools that formalize those social science theories as algorithms which can aid an observer who is not steeped in the local culture. While driven by practical problems, the objectives of the proposed work is not only to drive the development of new social science theories, but also to drive algorithmic advances in reasoning about joint probability distributions that arise from modeling uncertainties in human actions, speech, gestures, and intentions.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY16.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY16, the Division managed three new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase I contracts and one Phase II contract. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY16 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY16, the Division managed one new ARO (Core) HBCU/MI project and four new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The following PECASE recipients, previously nominated by this Division, were announced in this fiscal year by the White House. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Weakly Supervised Learning for Scalable Semantic Parsing. The objective of this PECASE, led by Professor Luke Zettlemoyer at the University of Washington, is to investigate the role of weak semantic parsing in question-answering systems and autonomous systems. Natural Language Processing (NLP) plays a central role in autonomous systems, whether they are simple automatic systems that conduct a survey or a full-bodied

robot that could participate in a team with human Soldiers in communicating with the outside world. NLP not only involves parsing sentences, which is compositional in nature, but also in breathing meaning to sentences. The latter depends on the context, where the meaning of propositions used not only depend upon surrounding sentences that either precede or follow a particular sentence, but also on the subject being discussed. While the past twenty years have seen a great increase in power of NLP due to the use of statistical techniques, true progress in NLP depends upon semantic interpretations. The PI proposes to consider "weak semantic parsing" -- the task of learning (i.e., bring statistical techniques to the table) in the context of assigning meaning to sentences that is dependent on the textual context of the sentence and on the subject matter of the sentence by investigating the notion of Combinatory Categorical Grammars (CCG), which allows for functions to be attached as semantic elements (in contrast to traditional parsing techniques that attach syntactic categories to phrases), thus allowing a polymorphic interpretation of linguistic elements.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY16, the Division managed nine new DURIP projects, totaling $1.5 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Big Mechanism Program

The Big Mechanism program attempts to understand conflicting information available in research literature on any big mechanism. The chosen area for the program is Cancer Biology, while the resulting techniques could be applied to a number of other mechanisms including climate change, with each piece of published work contributing a small portion of understanding to the big mechanism. The effort should lead to advances in the Natural Language Processing for automatically extracting information for scientific literature, advances in knowledge representation for signaling pathways with potential ambiguities in cancer biology, resolution of information from new publication against what is already known, and potential for advancement in explanation of causality of how cancer cells grow. This program is managed on behalf of DARPA through the Network Science Division, Intelligent Networks Program.

I. DARPA SIGMA Program

The SIGMA program is an effort to understand the issues associated with deploying a large sensor network for detection of nuclear threats in an urban environment. The concept of the program is to develop a very large network of sensors, that can be carried by people, but require no interaction. The program includes development of the sensors, communication networking via smart phone devices, and processing and fusing very large amounts of data. Communications and networking issues include security and privacy as well as dealing with data transfer from a large number of sensors. Portions of this program dealing with the sensor communications and networking as well as research into human factors dealing with technology adoption are managed on behalf of DARPA through the Network Sciences Division, Communications and Human Networks Program.

J. DARPA Communicating with Computers (CwC) Program

The goals of the DARPA Communicating with Computers program are to advance the state of the art in text and video analytics to the extent that a machine and its human operator can have the same mental model. This requires that the machine be able to understand the human intent, and that it can explain back, to the human, in ways that makes use of the context and prior knowledge. Three challenge problems have been chosen: (i) playing a game of blocks between humans and machines, (ii) a bicuration assistant that helps a human investigate knowledge representation of signaling pathways in cancer biology, and (iii) an author's assistant that could help a human write stories. This program is managed on behalf of DARPA through the Network Science Division, Intelligent Networks Program.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Network Sciences Division.

A. Scalable Temporal Network Models with Population Dynamics: Estimation, Simulation, and Prediction
Professor Zack Almquist, University of Minnesota - Minneapolis, Young Investigator Award

The objective of this research is to develop statistical techniques to inferentially test dynamic networks in which the population is in flux. In FY16, Professor Zack Almquist at the University of Minnesota developed statistical models to predict population (vertex) and link dynamics in social networks by expanding the family of Exponential Random Graph Models (ERGMs) used to model dynamic social network processes. Professor Almquist developed theory and software for performing dynamic network analysis, prediction, and simulation. In particular, he developed a vertex dynamics model to account for population dynamics (nodes entering and exiting the network over time) and their effects on network structure and network outcomes. Additionally, he developed the vertex model in combination with the Temporal Exponential Random Graph Models (TERGMs) to simultaneously account for dynamic populations and dynamic network structures as they evolve over time.

Professor Almquist tested and verified his joint vertex and link dynamic models using empirical data related to organizational collaboration networks for a natural disaster relief effort. With those data, he was able to demonstrate the predictability of the model with respect to the inherently dynamic nature of response teams, local and national organizations, and their engagement with each other throughout the duration of the crisis event. This dynamic vertex TERGM extension demonstrated considerable improvement over fixed vertex models with density prediction increasing from 0 to 75% (from 0 out of 12 time points for a fixed vertex model to 9 out of 12 for a dynamic vertex model (see FIGURE 1). The dynamic vertex model also demonstrated an increase in Krackhardt Connectedness prediction; from 1 out of 12 time points for a fixed vertex model to 7 out of 12 for a dynamic vertex model.
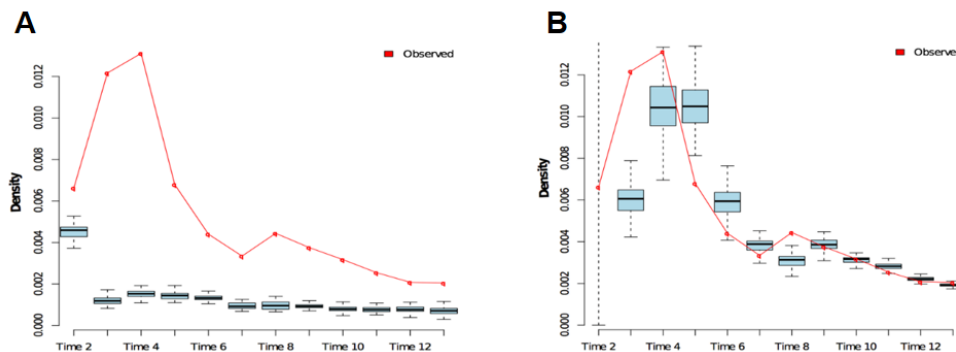

FIGURE 1

Longitudinal network density prediction with fixed and dynamic vertices. (A) Model without accounting for vertex dynamics does not successfully predict observed network density. (B) Model accounting for vertex dynamics successfully predicts 9 out of 12 time points within confidence interval.

This innovative work builds off the highly successful ERGM models to add elements that better handle missing data and temporal dynamics. This successful extension to the family of TERGMs pushes beyond the previous boundary requirement for a fixed set of vertices whereby all network nodes must be present at all time points of an evolutionary model. This new vertex dynamic model for social networks allows for statistically modeling not only link dynamics (changes in connections between the nodes), as was possible in the original TERGMs, but also vertex dynamics (nodes may enter and leave the model over time) in a single, combined model. Professor Almquist published his vertex dynamic models as R toolkits (open source statistical software) thereby making them accessible to the scientific community.

B. Adaptive Mobile Networking at the Tactical Edge
Professor Wei Gao, University of Tennessee, Single Investigator Award

The objective of this research is to investigate and exploit the close coupling between mobile communication networks and human social networks at the tactical edge by leveraging recent research in multi-genre networks. This analysis interprets warfighters' situational response to the heterogeneous battlefield contexts as their social dynamics, which are defined as the temporal and spatial variations of social relationships among warfighters, and are autonomously characterized from warfighters' contact patterns without manual inputs or configurations. However, due to the Disconnected, Intermittent, and Limited (DIL) network environment at the tactical edge which makes it hard to maintain persistent end-to-end wireless network connectivity among warfighters, there are many challenges of investigating, formulating, and exploiting such social dynamics for adaptive mobile networking, including: (i) the dynamics of warfighters' contact patterns need to be analytically and accurately formulated; (ii) a unified framework integrating models from multi-genre networks is needed to better characterize social dynamics among warfighters; and (iii) the global coordination and timely information exchange among warfighters is challenging due to the lack of end-to-end network connectivity, but are necessary for adaptive network decisions.

In FY16, Professor Gao developed a theoretical framework that incorporates prior tactical knowledge into the process of predicting warfighters' contacts with each other and hence improve the accuracy of contact prediction (see FIGURE 2).
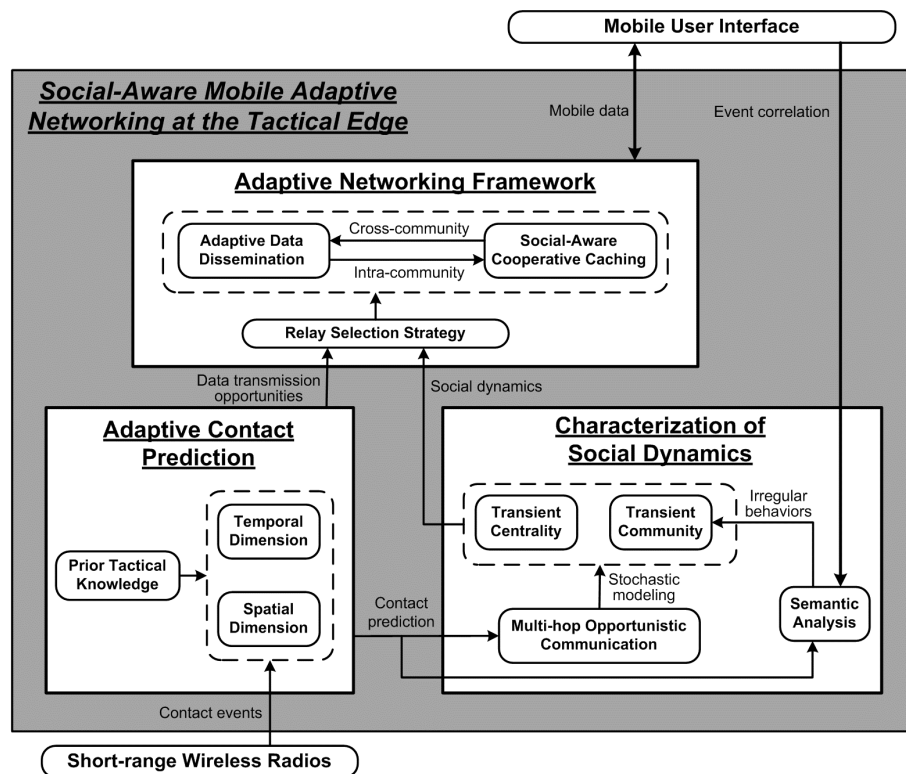

FIGURE 2

Theoretical bayesian framework for adaptive contact prediction.

The major difficulty that impairs the accuracy of such contact prediction at the tactical edge lies in the disconnection between the social relationship and contact patterns of warfighters. On one hand, social relationship among warfighters are initially assigned during the mission planning phase before their field deployment, in the form of tactical squads or mission teams. Such a relationship, therefore, could be partially fixed at all times and independent from the warfighters' actual behaviors in the theater. On the other hand, after deployment, warfighters at the tactical edge may autonomously self-organize themselves in different ways, in response to the situational contexts in the battlefield. These dynamic changes of their social relationship, then,

are implicitly reflected by their contact patterns and can be inferred with certain formalism of social network structures for contact prediction in the future. Existing social-aware contact prediction schemes, however, characterize the social relationship among warfighters solely from their in-situ contact patterns but ignore the prior knowledge of such social relationship before deployment. This ignorance will lead the results of contact prediction to deviate from the actual situation at the tactical edge, seriously impairing the performance of the mobile communication system. To bridge this gap, the Bayesian-based probabilistic inference framework combines both deployment information about the initial social relationship among warfighters and the in-situ contact patterns of warfighters after deployment. The framework was implemented and evaluated over realistic DIL network traces, and demonstrated that it outperforms existing contact prediction schemes.

C. Co-evolutionary Complex Networks: Dynamical Foundations, Influence, and Control
Professor Joshua Weitz, Georgia Institute of Technology, Single Investigator Award

The goal of this research is to develop theoretical methods, modeling approaches, and computational algorithms for co-evolutionary network dynamics, influence, and control. In FY16, research concentrated in the area of control of epidemics in complex networks by leveraging notions of individual awareness. Assuming individual awareness is an increasing function of the fraction of infected neighbors in a social network, the PI and his team characterized sufficient conditions for existence of a "metastable" or endemic state. A formalization of how awareness reduces the expectation of any epidemic metric (e.g. eradication time or total infections) on the space of sample paths was obtained. In related work, the researchers added individual decisions to notions of epidemic awareness. Specifically, they analyzed a model of disease spread dynamics over a contact network that depends on daily rational decisions of both healthy and sick individuals based on current risks of disease spread. They showed that preemptive measures of the sick individuals are crucial in determining whether the disease is eliminated or not. In contrast, the protective measures taken by the healthy individuals do not possess the efficacy of stopping a disease outbreak in the absence of empathetic actions by the sick individuals.

D. Crowd Sourcing for Scientific Discovery
Professor Carla Gomes, Cornell University, Single Investigator Award

The goal of this research is to combine the power of crowds, machine learning, and constraint satisfaction algorithms to design new unheard of materials. High-throughput materials discovery involves the rapid synthesis measurement, and characterization of many different but structurally related materials. A central problem in materials discovery, the phase map identification problem, involves the determination of the crystal structure of materials from materials composition and structural characterization data. In FY16, the PI developed Phase-Mapper, a novel solution platform that allows humans to interact with both the data and products of artificial intelligence algorithms, including the incorporation of human feedback to constrain or initialize solutions. Phase-Mapper is compatible with any spectral demixing algorithm, including their novel solver, AgileFD, which is based on convolutive non-negative matrix factorization. AgileFD allows materials scientists to rapidly interpret XRD patterns, and can incorporate constraints to capture the physics of the materials as well as human feedback. The PI used three solver variants with previously proposed methods in a large-scale experiment involving 20 synthetic systems, demonstrating the efficacy of imposing physical constraints using AgileFD. Since the deployment of Phase-Mapper at the Department of Energy's Joint Center for Artificial Photosynthesis (JCAP), thousands of X-ray diffraction patterns have been processed and the results are yielding discovery of new materials for energy applications, as exemplified by the discovery of a new family of metal oxide solar light absorbers, among the previously unsolved Nb-Mn-V oxide system. Phase-Mapper is also being deployed at the Stanford Synchrotron Radiation Lightsource (SSRL) to enable phase mapping on datasets in real time.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Mitigation of Cyber Attacks on Sensor Networks
Investigator: Professor Rick Blum, Lehigh University, Single Investigator Award
Recipient: Netizen, Inc.

Professor Rick Blum has developed a novel framework that will allow a sensor network to estimate the desired parameter vector at the fusion center while under cyberattack. They have analyzed both spoofing attacks (changing measured data) and man-in-the middle attacks (changing digital data) on the sensor. The algorithms simultaneously detect sensors under attack, and estimates both the attack parameters and desired parameter vector for both spoofing attacks (modifying measured signal) and man-in-middle attacks (modifying the transmitted quantized data). This is achieved by analysis of the Fisher information matrix to understand lower bounds of estimation performance. These new algorithms have applicability in many sensor network applications, including traditional wireless sensor networks and smart grids. Professor Blum has received funding from the state of Pennsylvania to work with Netizen, Inc. to transition this research with applications to attacks on the IEEE 1588 network timing synchronization. The IEEE 1588 protocol sends messages between the nodes that can be used to estimate the offset between the clocks at two nodes in order to synchronize them.

B. Spatio-Temporal Game Theory
Investigator: Professor Milind Tambe, University of Southern California, MURI Award
Recipient: County of Los Angeles, CA

Predicting, tracking, and validating the spread of information through a community is relevant to health care professionals and the U.S. Army,. Typically, over a long period of time, an organization may be able to map the social network of its consumers and would know how to send a product-focused message. However, when such information is lacking, it is necessary to concomitantly send out information, measure how it spreads, and adjust the message in order to spread the information as widely as possible. Professor Tambe's team has been working with Los Angeles County in spreading educational information about AIDS, and appropriate prevention mechanisms, among the homeless population of L.A. County. The PI devised a new algorithm to map out the social network structure and the efficacy of a campaign, as a game theoretical algorithm, and a system, based on this algorithm, has been deployed by L.A. County.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Distributed High Performance Algorithms for Operation of MANETs
Professor Javad Ghaderi, Columbia University, Single Investigator Award

Mobile Ad hoc Networks (MANETs) that can operate in a distributed fashion, without infrastructure, and without the need of a central coordinator, are especially suitable for rapid deployment and autonomous communication. However, traditional networking and information-theoretic approaches require substantial complexity and coordination to deliver high quality communications with guaranteed on-time packet delivery over such networks, and hence are not suitable for distributed operation.

It is anticipated that in FY17, the PI will create low-complexity distributed algorithms in which the individual nodes can operate autonomously and can efficiently share the wireless medium in a distributed fashion. Specifically, the following are the main objectives of the research: (i) investigate low-complexity randomized combined physical layer/medium access distributed control to efficiently manage interference using scheduling and power/rate spaces; (ii) develop deadline-based versions of current distributed algorithms which achieve low complexity as well as packet delivery within a guaranteed deadline; and (iii) develop implementation in the presence of channel fading and multi-hop traffic in order to validate the research in a realistic scenario.

The approach is guided by three significant breakthroughs in recent years: (i) the development of Queue-based Carrier Sense Multiple Access (Q-CSMA), which is a simple random access algorithm in which nodes make transmission decisions based on limited local information and can still match the optimal throughput performance of the centralized algorithm, (ii) significant recent progress in deadline-based mechanisms for packet transmission that ensure on-time delivery of packets, and (iii) exciting new physical-layer strategies, such as interference alignment, successive interference cancellation, and other cooperative schemes that can boost throughput. Each of these developments focuses on one aspect of performance, namely, either throughput, delay, or complexity, but not all three aspects together. This research will use a joint physical-layer/networking perspective to design algorithms that can achieve low complexity, high throughput, and small delay.

B. Quantifying Cognitive Factors in Online Social Behavior
Professor Kristina Lerman, University of Southern California, Single Investigator Award

The objective of this research is to measure the impact of cognitive factors on individual choices and the collective outcomes of those choices. It is anticipated that in FY17, this research will focus on understanding how people make decisions to allocate attention and the role that cognitive factors play in these decisions. Of specific focus will be the biases important in online interactions, such as message position bias, social influence bias, and affect biases. The PI will explore how cognitive biases interact with social network structures to give rise to the observed patterns of social influence and the spread of information online.

Professor Lerman will test and validate her hypotheses with empirical data from a variety of sources including Stack Exchange (an online Question and Answer forum), reddit (a social media platform for collectively sharing and rating news stories), and experimentally collected data. Taking a "big data" approach, Professor Lerman will address such research questions as: How do cognitive biases affect individual judgments and collective performance online? How does cognitive load affect online behavior? What are the impacts of information overload on performance? This innovative, human dimension research will extend current theory by providing important insights and structured understanding of information processing under high cognitive load conditions. Additionally, if successful, this research will provide quantitative results demonstrating the limitations around human cognitive processing of online information.

C. Quantifying Network Controllability and Observability using Optimal Control and Estimation Metrics
Professor Tyler Summers, University of Texas - Dallas, Single Investigator Award

Recently there has been an increasing interest in characterizing the number of nodes needed to ensure structural controllability in a network of dynamical systems. Traditional definitions of controllability seem ill-suited in this context as controllability may be achieved with only a small subset of nodes but large amounts of energy. Professor Summers has created a novel approach by optimizing the value function of a general (open-loop) control problem over the sets of nodes that are under control. When the value function is submodular (i.e. adding a new node to the existing set of nodes under control provides decreasing marginal value), Professor Summers has shown that the approach provides a computationally tractable means for characterizing network controllability.

It is anticipated that in FY17, Professor Summers will extend this line of work to characterizing controllability with closed-loop strategies. This approach with be tested on several application domains including surveillance and reconnaissance with multi-robot teams, neuronal brain networks, and power grids.

D. Steering T-Cell Adaptation Using Opponent Exploitation Algorithms
Professor Tuomas Sandholm, Carnegie Mellon University, Single Investigator Award

Professor Tuomas Sandholm is investigating the use of Algorithmic Game Theory techniques to devise therapeutic strategies, based on reasoning about the biochemical reaction associated with adaptation by T-Cells, to steer abnormal cells (such as cancer cells) to mutate to benign state. The research will involve designing solutions to large mathematical games that would arise in modeling the interactions between T-Cells, pathogens, and potential treatment plans. It is anticipated that in FY17, the research will uncover the "games" that arise in this context and on driving research in biology to reduce uncertainty in knowledge of dynamics of interacting biochemical agents.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Purush Iyer
Division Chief
Program Manager, Intelligent Networks

Dr. Alfredo Garcia
Program Manager, Multi-Agent Network Control

Dr. Edward Palazzolo
Program Manager, Social and Cognitive Networks

Dr. Robert Ulman
Program Manager, Communication and Human Networks

B. Directorate Scientists

Dr. Randy Zachery
Director, Information Sciences Directorate

Dr. Bruce West
Senior Scientist, Information Sciences Directorate

Ms. Anna Mandulak
Contract Support

C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 11: PHYSICS DIVISION

I.   OVERVIEW

As described in CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication ARO in Review 2016 is to provide information on the programs and basic research supported by ARO in FY16, and ARO's mission to create basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Physics Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY16.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Physics Division supports research to discover exotic quantum and extreme optical physics. The Division promotes basic research that explores frontiers where new regimes of physics promise unique function. Examples such as ultracold molecules, complex oxide heterostructures, attosecond light pulses, and quantum entanglement all represent areas where the scientific community's knowledge must be expanded to enable an understanding of the governing phenomena. The results of this research will stimulate future studies and help to keep the U.S. at the forefront of research in physics.

2. Potential Applications. Research managed by the Physics Division will provide a scientific foundation upon which revolutionary future warfighter capabilities can be developed. The Division's research is focused on studies at energy levels suitable for the dismounted Soldier: the electron Volt and milli-electron Volt range. In the long term, the discoveries are anticipated to impact warfighter capabilities in the area of Command, Control, Communications, Computers, Intelligence, Surveillance, and Reconnaissance (C4ISR). Research advances in the Division can be readily visualized to impact sensor capabilities for increased battlespace awareness and Soldier protection, enhanced navigation, ultra-lightweight optical elements and energy-efficient electronics for decreased Soldier load, increased Soldier awareness, and advanced computational capabilities for resource optimization and maximal logistical support.

3. Coordination with Other Divisions and Agencies. To meet the Division's scientific objectives and maximize the impact of discoveries, the Physics Division coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multidisciplinary research topics, and evaluate the effectiveness of research approaches. For example, research co-funded with the Mathematical Sciences Division seeks coherent-feedback quantum control of collective hyperfine spin dynamics in cold atoms. Collaborative research with the Electronics Division is also underway with a goal of understanding high frequency responsiveness of magnetic materials and the engineering of agile radio frequency device concepts. The Division coordinates its research portfolio with AFOSR and DARPA in pursuit of forefront research involving ultracold molecules and optical lattices. The Division also coordinates certain projects with Intelligence Advanced Research Projects Activity (IARPA) and other government agencies. These interactions promote a synergy among ARL and DoD agencies, and improve the quality of the Division's research areas.

In addition, the Division's research portfolio will reveal previously unexplored avenues for new Army capabilities while also providing results to support (i) the Materials Research Campaign's goals to determine how quantum processes could be harnessed for quantum memory and secure communication, and to explore and exploit recent advances in interface physics between unique materials such as topological insulators and their quantum mechanical properties, (ii) the Information Sciences Campaign's goal to explore techniques, architectures, and properties that take advantage of the quantum and related effects for transmitting information,

and (iii) the Sciences for Lethality-and-Protection Campaign's goal to identify, exploit, and protect against the effects of directed and non-directed application of energy.

B. Program Areas

The Physics Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY16, the Division managed research within these four Program Areas: (i) Atomic and Molecular Physics, (ii) Condensed Matter Physics, (iii) Optical Physics and Fields, and (iv) Quantum Information Science. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term aspirations that collectively support the Division's overall objectives.

1. Atomic and Molecular Physics. The goal of this Program Area is to study the quantum properties of atoms and molecules and advance a fundamental understanding of exotic quantum behavior. When a gas of atoms is sufficiently cooled, the quantum nature dominates and the atoms behave wave-like rather than a cloud of distinct particles. Accordingly, experiments that were once the sole purview of optics are now possible with matter: interference, lasing, diffraction and up/down-conversion, to name a few. This Program Area explores these concepts with an eye toward enabling new opportunities, such as novel quantum chemistry and atomic devices that exploit quantum behavior. The specific research Thrusts within this Program Area are: (i) State-dependent Quantum Chemistry, (ii) Atomtronics, and (iii) Non-equilibrium Many-body Dynamics. Ultracold gases can be trapped in 1D, 2D, or 3D standing optical waves enabling the exploration of novel physics, quantum phase transitions, and mechanisms operative in condensed matter. In optical lattices, one can also create a new "electronics", called atomtronics, based on atoms and molecules having statistics, mass, charge, and many additional handles not available in conventional electronics. The State-dependent Quantum Chemistry Thrust is not focused on synthesis but rather on the underlying *mechanisms*, such as electronic transport, magnetic response, coherence properties (or their use in molecule formation/selection), and/or linear and nonlinear optical properties. While the notion of taking objects held at sub-Kelvin temperatures onto a battlefield may seem irrational, dilute atomic gases can be cooled to nano-Kelvin temperatures without cryogens (e.g., liquid helium) by using magnetic traps and lasers. The long-term applications of this research are broad and include ultra-sensitive detectors, time and frequency standards, novel sources, atom lasers and holography, along with breakthroughs in understanding strongly-correlated materials and to design them from first principles.

2. Condensed Matter Physics. The objective of this Program Area is to discover and characterize novel quantum phases of matter at oxide-oxide interfaces and at the surfaces and interfaces of topological insulators. Recent studies have shown that interfaces can support quantum phases that are foreign to the bulk constituents. Furthermore the bond angles and bond lengths in complex oxides are controllable at interfaces. In general the interface provides a mechanism for potentially controlling lattice, orbital, spin and charge structure in ways that are not possible in bulk, single phase materials. If these degrees of freedom can be engineered in ways analogous to charge engineering in semiconductors, it will present new opportunities for the development of advanced technologies utilizing states beyond just charge. Topological insulators represent a relatively recent discovery of a state of matter defined by the topology of the material's electronic band structure rather than a spontaneously broken symmetry. What is unique about this particular state is that unlike the quantum Hall state—which is also characterized by a topology,—it can exist at ambient conditions: room temperature and zero magnetic field. In general, discovering, understanding, and experimentally demonstrating novel phases of matter in strongly correlated systems will lay a foundation for new technological paradigms. Nanometer-scale physics, often interpreted as a separate field, is also of interest as confined geometries and reduced dimensionality enhance interactions between electrons leading to unusual many-body effects. A critical component for gaining new insights is the development of unique instrumentation and this program supports the construction and demonstration of new methods for probing and *controlling* unique quantum phenomena.

3. Optical Physics and Fields. The goal of this Program Area is to explore the formation of light in extreme conditions and the novel manipulation of light. Research is focused on physical regimes where the operational physics deviates dramatically from what is known. The specific research thrusts within this Program Area are Extreme Light and Meta-optics. In addition, any fundamental fields that carry energy and information are of interest. The Extreme Light thrust involves investigations of ultra-high intensity light, light filamentation, and

femtosecond/attosecond laser physics. High-energy ultrashort pulsed lasers have achieved intensities of 10^{22} W/cm^2. Theoretical and experimental research is needed to describe and understand how matter behaves under these conditions, including radiation reaction and spin effects, from single particle motion to the effects in materials, and how to generate these pulses and use them effectively. One consequence of ultra-high power lasers is light filamentation, which creates a supercontinuum of coherent light across the visible spectrum. Ultra-short intense pulses can be utilized to develop attosecond pulses by combining them with high harmonic generation. Potential long-term applications include imaging through opaque materials, laser pulse modulation, "observing" electron dynamics, and even controlling electron dynamics. Research in the Meta-optics thrust includes studies of optical angular momentum (OAM) beams, interactions with metamaterials, and novel optical physics. An example is the study of OAM beams and how they interact with metamaterials, or how they can be used to induce new kinds of interactions or physics. Another area of interest regards overcoming losses in metamaterials. Cloaking is a well-known idea, but losses and the dispersion must be overcome before this is a reality in the practical sense. In addition, other fields which may be used in place of electrodynamics are of interest to this program. Examination of parity-time symmetric optics is being considered to understand and compensate for loss; topological photonics, Chern number calculation, and topological interactions are also of interest. More generally, research in supersymmetric optics and its relation to topological effects are of interest.

4. Quantum Information Science. The objective of this Program Area is to understand, control, and exploit nonclassical, quantum phenomena for revolutionary advances in computation, sensing and secure communications. Three major Thrusts are established within this program: (i) Foundational Studies, (ii) Quantum Computation and Communication, and (iii) Quantum Sensing and Metrology. Research in the Foundational Studies Thrust involves experimental investigations of the wave nature of matter, including coherence properties, decoherence mechanisms and mitigation, entanglement, nondestructive measurement, complex quantum state manipulation, and quantum feedback. The objective is to ascertain current limits in creating, controlling, and utilizing information encoded in quantum systems in the presence of noise. Of particular interest is the demonstration of the ability to manipulate quantum coherent states on time scales much faster than the decoherence time, especially in systems where scalability to many quantum bits and quantum operations is promising. Quantum Computation and Communication entails experimental demonstrations of quantum logic performed on several quantum bits operating simultaneously, with demonstrations of quantum feedback and error correction for multiple quantum bit systems are also of interest. There is particular interest in developing quantum algorithms for solving NP-complete problems for use in resource optimization and in developing quantum algorithms to simulate complex physical systems. Research in the Quantum Sensing and Metrology Thrust involves studying the transmission of information through quantum entanglement, distributed between spatially separated quantum entities. Long-range quantum entanglement, entanglement transfer among different quantum systems, and long-term quantum memory are of interest. An emerging field of interest is quantum sensing and metrology using small entangled systems. Entanglement provides a means of exceeding classical limits in sensing and metrology and the goal is to demonstrate this experimentally.

C. Research Investment

The total funds managed by the ARO Physics Division for FY16 were $77.6 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY16 ARO Core (BH57) program funding allotment for this Division was $7.1 million and $1.0 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $7.5 million to projects managed by the Division. The Division also managed $8.4 million of Defense Advanced Research Projects Agency (DARPA) programs, and $50.9 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.1 million for contracts. Finally, $1.8 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which included $0.2 million of the Division's total ARO Core (BH57) funds, in addition to funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY16 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY16 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY16, the Division awarded 21 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Francois Amet, Appalachian State University; *Topological Electronic Phases In Hybrid Superconductor - Quantum Hall Effect Structures*

- Professor Meigan Aronson, Texas A&M University; *Superconducting Quantum Critical Points In Topological Half-Heusler Compounds*

- Professor Brian DeMarco, University of Illinois - Urbana-Champaign; *Localization, Excitation, and Relaxation in Disordered Atomic Hubbard Models*

- Professor David DeMille, Yale University; *Laser Cooling and Trapping of Diatomic Molecules*

- Professor Gleb Finkelstein, Duke University; *Search For Novel Topological Phases And Excitations In Superconductor - Quantum Hall Hybrid Samples*

- Professor Benjamin Lev, Stanford University; *Computing with Neuromorphic Dissipative Quantum Phase Transitions*

- Professor Charles Marcus, University of Copenhagen; *Voltage-Controlled Semiconductor Nanowire-Based Superconducting Qubits*

- Professor Nai Phuan Ong, Princeton University; *Transport and Tunneling Experiments on Dirac and Weyl Semimetals*

- Professor Sahin Ozdemir, Washington University; *Optomechanics in Parity-Time Symmetric Photonic Structures*

- Professor Viktor Podolskiy, University of Massachusetts - Lowell; *Plasmon-Phonon And Plasmon-Magnon Interaction In Metamaterials: Multi-Physics Paradigm For Acousto-Optical And Magneto-Optical Technologies*

- Professor Enrico Rossi, College of William and Mary; *Topological Heterostructures*

- Professor Mark Saffman, University of Wisconsin - Madison; *Hybrid Atom-Superconductor Quantum Interface*

- Professor Vito Scarola, Virginia Polytechnic Institute and State University; *Chiral Spin Liquids and Other Topological Phases of Cold Atoms and Molecules in Optical Lattices*
- Professor Monika Schleier-Smith, Stanford University; *Quantum Simulation of Frustrated Magnets by Rydberg Dressing*
- Professor Gennady Shvets, University of Texas - Austin; *Investigations of Photonic Topological Structures Based on Metallic and All-Dielectric Metamaterials*
- Professor Alexander Thomas, University of Michigan - Ann Arbor; *Radiation Reaction in Intense Laser Interactions with Relativistic Electrons and Nonlinear Compton Scattering*
- Professor Joseph Thywissen, University of Toronto; *Dynamics and Spin Transport of Ultracold Fermions*
- Professor Anthony Vamivakas, University of Rochester; *Quantum Vacuum Modes as a Probe*
- Professor Kevin Webb, Purdue University; *The Optomechanical Response of Nanostructured Materials*
- Professor David Weiss, Pennsylvania State University; *Non-Equilibrium Dynamics In Optical Lattices*
- Professor Amir Yacoby, Harvard University; *Contacting the Quantum Anomalous Hall State*

2. Short Term Innovative Research (STIR) Program. In FY16, the Division awarded one new STIR project to explore high-risk, initial proof-of-concept ideas. The following PI and corresponding organization was the recipients of the new-start STIR award.

- Professor Natalia Litchinitser, State University of New York (SUNY) at Buffalo; *Nonlinear Topological Surface States in Meta-Crystals*

3. Young Investigator Program (YIP). In FY16, the Division awarded two new YIP projects to drive fundamental research in areas relevant to the current and future Army. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor Liang Feng, State University of New York (SUNY) at Buffalo; *Robust Light State and Transport by Quantum Phase Transition in Non-Hermitian Photonic Materials*
- Professor Javad Shabani, CUNY - City College of New York; *Epitaxial Superconductor-Semiconductor Two-Dimensional Systems: A New Platform For Quantum Computation*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY16 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Decoherence Mechanisms in Superconducting Qubits 2*; University of Maryland - College Park; April 21-22, 2016
- *2016 Strongly Correlated Electron Systems Gordon Research Conference*; Mt. Holyoke, MA; 26 June - 1 July 2016

5. Special Programs. In FY16, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded two new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in CHAPTER 2: *PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These projects constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Transformation Optics - Exploring New Frontiers in Optics. This MURI began in FY09 and was awarded to a team led by Professor David Smith at Duke University. The objective of this research is to explore new frontiers in optics made possible by the discovery of negative-index materials (NIMs), with additional work to fabricate tunable metamaterials on specific substrates.

In current optics technology, light refracts (bends) as it passes from one material to another. By curving a surface, such as a lens, refraction is used to focus light. Unfortunately this process loses some of the information contained within the light. As a result, current lenses, such as those used in a microscope, essentially prevent the user from viewing objects smaller than the wavelength of visible light (*i.e.*, limited to about 0.5 micrometers). NIMs can be designed through the use of metamaterials (*i.e.*, artificial materials engineered to provide specific properties not available in naturally-made structures) or by the construction of photonic crystals.

A prior MURI award (FY06-FY11) that was managed by the ARO Physics Division and led by Professor Vlad Shalaev at Purdue University, pioneered many early discoveries and advances in NIMs that in turn manifested a new field in optics termed transformation optics. By combining the negative refraction of NIMs with an index of refraction that varies spatially and temporally, optical materials can be designed to have properties not possible with conventional optics. This MURI team, which includes Professor Shalaev as a co-investigator, is exploring this new frontier in physics. The researchers are investigating methods of controlling light by design, routing it where conventional optics cannot. For example, with transformation optics, light of a particular wavelength can be bent around an object rendering the object invisible at that wavelength. This has already been demonstrated in the microwave band but has not yet been shown at the wavelengths of visible light. The second objective is the development of a flat hyperlens: a lens that is flat on both sides and not only magnifies but also resolves nanometer-scale features. This lens could provide a resolution at least an order of magnitude beyond the diffraction limit of conventional optics. Not only can transformation optics be used to bend light around an object but it can also be used to bend light toward an object. The third major objective is to design materials accordingly such that light from all directions is concentrated on a single detector. These concentrators could revolutionize optical sensors and solar energy collection as its omnidirectional nature eliminates the requirement of moving parts.

2. Atomtronics: an Atom-Analog of Electronics. This MURI began in FY10 and was awarded to a team led by Professor Ian Spielman of the University of Maryland. The objective of this MURI is to explore and understand the concepts of atom-based physics, beginning with the rich and fundamental physics discoveries already revealed with cold atoms systems and to investigate the concepts required for future device applications.

Atom-based physics studies (atomtronics) are analogous to, but will go beyond, the fundamental twentieth century studies regarding the properties of electrons (*i.e.*, electronics) that enabled the electronics revolution. Solid-state electronics, heralded by the transistor, transformed both civilian and military culture within a generation. Yet there is only a single kind of electron: its mass, charge and spin (and thus quantum statistics as well) are unalterable. Atoms on the other hand, come with different masses, can have multiple charge states, and have a variety of spin and other internal quantum states. Accordingly, studies in atomtronics aim to understand an atom-based physics rather than electron-based device physics. Breakthroughs in cold atom physics and degenerate quantum gases presage this new kind of device physics. That cold atom science has resulted in atomic analogies to other technologies, such as optics and lasers, suggests that the same may be repeated with electronics. Very good analogies of solids and junctions can be made with trapped atoms. It is now well-known how one, two and three dimensional structures with essentially any lattice geometry can be formed in cold, trapped atoms. A few theory papers have pointed the way to simple devices.

The most apparent, but not necessarily the only approach to atomtronics, is through optical lattices, where Bloch's theorem holds. Band structure is the first basis on which physicists understand traditional (electronic) metal, insulator, and semiconductor behavior. Interaction and disorder modify this and exploration of Mott-like and Anderson-like insulators and transitions are envisioned as well. Doping can be mimicked by modifying atoms in certain wells or by locally modifying the lattice potential, which can be done with additional optical fields. Such defects could be deeper or shallower wells, or missing or additional sites. Recent breakthroughs involving three dimensional optical lattices and the loading of atoms into lattices with reasonably long lifetimes have set the stage for atomtronics.

Atomtronics researchers are focused on two key themes devices and connections. The envisioned analogs to devices can be described as those that perform actions under external control and those that can be cascaded. The researchers will explore spin-orbit coupling in atomic systems in an effort to exploit new degrees of freedom in "spintomic" device concepts as well as novel reversible logic via cascaded spintomic gates. In addition, researchers will investigate far from equilibrium regimes, which is not possible in condensed matter systems due to the residual phonon interactions at finite temperatures. The second theme centers on connections and is split

between analogs to electronics and novel interfacing. The research team use the superfluid properties of ultracold atoms confined in rings to create circuits. These small circuits interact with lasers to demonstrate an analogous SQUID device. Finally the researchers are exploring novel interfacing by trapping atoms with evanescent waves along ultrathin optical fibers. It is hoped that this technique will allow several devices to be coupled while remaining isolated from the environment.

3. Multi-Qubit Enhanced Sensing and Metrology. This MURI began in FY11 and was awarded to a team led by Professor Paola Cappellaro at the Massachusetts Institute of Technology. The objective of this research is to explore and demonstrate imaging, sensing and metrology beyond the classical and standard quantum limits by exploiting entangled multi-qubit systems.

Precision measurements are among the most important applications of quantum physics. Concepts derived from quantum information science (QIS), such as quantum entanglement, have been explored for the past decade to enhance precision measurements in atomic systems with potential applications such as atomic clocks and inertial navigation sensors. QIS has also enabled the development of new types of controlled quantum systems for the realization of solid-state qubits. These systems could potentially be used as quantum measurement devices such as magnetic sensors with a unique combination of sensitivity and spatial resolution. However, progress towards real-world applications of such techniques is currently limited by the fragile nature of quantum superposition states and difficulties in preparation, control and readout of useful quantum states. The power of entangled and squeezed states for quantum sensing lies in their sensitivity to the external parameter to be measured.

This MURI aims to overcome three major obstacles to practical quantum sensor operation: the difficulty to experimentally create desired entangled many-qubit input states to the sensing device, the fragility of the states during signal acquisition, and low fidelity of the readout process. The results of this research may ultimately lead to dramatic improvements in imaging, sensing, and metrology.

4. Light Filamentation. This MURI began in FY11 and was awarded to a team led by Professor Martin Richardson at the University of Central Florida. The objective of this research is to establish the underlying qualitative and quantitative understanding of the physical phenomena associated with light filaments in order to create and control the filaments and their associated unique properties.

A light filament is a novel form of propagating energy that is a combination of a laser beam and plasma. A light filament has three characteristics that make it unlike any other form of energy, and also make it ideal for remote detection of trace materials. Like laser light, a light filament is coherent. However, unlike laser light, it undergoes wavelength dispersion as the beam propagates, creating a coherent beam with wavelengths across the entire visible spectrum. Since the beam contains laser radiation at every wavelength, it is sometimes called a super-continuum or white laser. The continuum has a high UV content, which makes it of interest for remote chemical spectroscopy. Finally, by beating the diffraction limit, a light filament does not diverge in space. Unlike any other form of energy propagation, a light filament can be as small at a distant target as it was when it was created. Light filaments are formed when intense laser pulses are focused down, due to the nonlinearity of the air (the Kerr effect), to about 100 microns. At this point, the intense field ionizes, creating a plasma. The plasma stops the self-focusing and equilibrium is reached. The complex interaction of the plasma and electromagnetic field creates these unique properties of light filaments. Although light filaments are extremely rich in phenomena for potential applications, the complex interaction of optical, plasma, and electromagnetic behaviors is poorly understood.

The research team is attempting to create light filaments and understand and predict light filament propagation characteristics, length, interactions with matter, and electromagnetic interactions. If successful, this research could ultimately lead to controllable light filaments that would revolutionize remote detection and imaging through clouds, creating a new ability in standoff spectroscopic detection.

5. Surface States with Interactions Mediated by Bulk Properties, Defects and Surface Chemistry. This MURI began in FY12 and was awarded to a team led by Professor Robert Cava at Princeton University. This project is exploring the recently-discovered class of materials known as topological insulators.

A topological insulator is a material that behaves as a bulk insulator with a surface that is metallic (permitting the movement of charges on its surface) due to the fundamental topology of the electronic band structure. This topological property separates it from nearly every other known phase of matter. Instead of a phase being due to a broken symmetry (such as results in crystalline, magnetic, superconducting, etc. phases), the property of

metallic surfaces results from a transition between two topologically distinct phases: trivial and non-trivial. This is a parallel to the quantum Hall effect which also results from topology but it has two dramatic enhancements. First, it is not limited to two dimensions, and second, the physics should be able to survive to ambient conditions if materials are sufficiently clean. The quantum Hall effect and related phenomena require ultra-low temperatures and high magnetic fields to induce them. Topological insulators do not.

The objective of this research is to advance the discovery, growth, and fabrication of new bulk- and thin-film-based topologically-stabilized electronic states in which electron-electron interactions play a significant role. The researchers are bringing strong materials science, chemistry and surface science approaches to bear on the study of the novel properties of topological insulators. Research in this area has great potential for long-term benefits for the Army, such as electronically-controlled magnetic memory and low-power electronics.

6. High-Resolution Quantum Control of Chemical Reactions. This MURI began in FY12 and was awarded to a team led by Professor David DeMille at Yale University. This MURI is exploring the principles of ultracold molecular reaction, where chemical reactions take place in the sub-millikelvin temperature regime. This research is co-managed by the Chemical Sciences and Physics Divisions.

The study of ultracold molecular reactions, where chemical reactions take place in the sub-millikelvin temperature regime, has emerged as a new field in physics and chemistry. Nanokelvin chemical reactions are radically different than those that occur at "normal" temperatures. Chemical reactions in the ultracold regime can occur across relatively long intermolecular distances, and no longer follow the expected (Boltzmann) energy distribution. The reactions become heavily dependent on nuclear spin orientation, interaction strength, and correlations. These features make them a robust test bed for long-range interacting many-body systems, controlled reactions, and precision measurements.

The objectives of this MURI are to develop a fundamental understanding of the nature of molecular reactions in the nano-K temperature regime and to extend the cooling technique previously demonstrated by Professor DeMille[1] (through a previous ARO award) to other molecular candidates. The researchers are focused on the implementation of novel and efficient laser cooling techniques of diatomic molecules, and to understand the role of quantum effects, including the role of confined geometries, on molecules that possess vanishingly-small amounts of thermal energy. This research could lead to new devices or methods that explicitly use quantum effects in chemistry, such as the precision synthesis of mesoscopic samples of novel compounds, new avenues for detection of trace molecules, and a new understanding of combustion and atmospheric chemical reactions.

7. Non-equilibrium many-body dynamics. This MURI began in FY13 and was awarded to a team led by Professor Cheng Chin at the University of Chicago. The goal of this MURI is to study fundamental non-equilibrium dynamics using cold atoms in optical lattices.

Dynamics far from equilibrium is of great importance in many scientific fields, including materials science, condensed-matter physics, nonlinear optics, chemistry, biology, and biochemistry. Non-equilibrium dynamics recently has taken on significance in atomic physics, where new tools will enable breakthroughs. In particular, optical lattice emulation is allowing one to gain insight, and potentially solve, traditionally intractable problems, including those out of equilibrium. Breakthroughs in other disciplines are also enabling a new look at non-equilibrium. In materials science, a recent pump-probe experiment enabled dynamical control of material properties.[2] Another example is in biochemistry, in determining the role that non-equilibrium phase transitions play in driven biochemical networks, e.g., canonical phosphorylation-dephosphorylation systems with feedback that exhibit bi-stability.[3-4] Despite the ubiquitous nature of non-equilibrium dynamics, little scientific progress has been made due to the many challenges, including the difficulty in finding many-body systems that remain far from equilibrium on experimentally accessible time scales.

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[1] Shuman ES, Barry JF, DeMille D. (2010). Laser cooling of a diatomic molecule. *Nature*. 467:820–823.

[2] Goulielmakis E, Yakovlev VS, Cavalieri AL, et al. (2007). Attosecond control and measurement: lightwave electronics. *Science*. 317:769-775.

[3] Qian H. (2006). Open-system nonequilibrium steady state: statistical thermodynamics, fluctuations, and chemical oscillations. *J. Phys. Chem. B*. 110:15063-15074.

[4] Ge H and Qian H. (2011). Non-equilibrium phase transition in mesoscopic biochemical systems: from stochastic to nonlinear dynamics and beyond. *J. R. Soc. Interface*. 8:107-116.

The objective of this MURI project is to discover how many-body systems thermalize from non-equilibrium initial states, and explore the dynamics of far-from-equilibrium systems. Given that non-equilibrium dynamics plays an important role in many scientific and engineering areas, such as quantum sensing and metrology, atomtronics, and quantum chemistry, this research could ultimately lead to the development of dynamic materials, and devices for improved computation, precision measurement, and sensing.

8. Ultracold Molecular Ion Reactions. This MURI began in FY14 and was awarded to a team led by Professor Eric Hudson at the University of California - Los Angeles. The goal of this MURI is to design, create, and exploit molecular ion traps to explore precision chemical dynamics and enable the quantum control of ultracold chemical reactions. This research is co-managed by the Chemical Sciences Division.

Investments quantum computing and precision metrology have led to the development of molecular ion trap technology. These advances provide scientific opportunities that could be exploited to enable new methods for the study and control of chemical reactions. Recent scientific breakthroughs have been achieved in ultra-cold chemistry with neutrals, suggesting that ion chemistry would provide similar opportunities for an emerging new field. In addition, work in quantum information has led to the development of new types of arrayed micro-fabricated ion traps. Ion trap technology adds novel capabilities to molecular ion research, enabling new research opportunities in materials science, condensed-matter physics, chemistry, and biochemistry. In particular, ion traps offer dramatic improvements in chemical sensing at the single-ion level. Compared with molecular neutrals, trapped molecular ions offer interaction times much longer than what is possible in beam experiments; state preparation and readout is potentially cleaner; and Coulomb interactions with co-trapped atomic ions allow for general species-independent techniques.

The objective of this research is to develop and create molecular ion traps to exploit long interrogation time to study molecular ion chemistry, utilize extended interaction times and dipolar interactions in novel quantum control scenarios, improve chemical sensing using single-ion detection, and integrate the traps with various detectors. This research could ultimately leave to dramatically improved methods for creating and studying quantum dots, energetic compounds, biological reactions, and tools for detection of trace molecules.

9. Engineering Exotic States of Light with Superconducting Circuits. This MURI began in FY16 and was awarded to a team led by Professor Andrew Houck at Princeton University. The goal of this MURI is to initiate significant new experimental and theoretical explorations to harness recent breakthroughs in superconducting systems and to demonstrate useful new states of light that can be brought to bear on broader goals in sensing, measurement, simulation, and computation. This research is co-managed with the Electronics Division. If successful, this research may lead to new tools for metrology, could provide key insight into non-equilibrium quantum systems, and will provide new resources for quantum communication and sensing.

Quantum optics, particularly in the domain of cavity quantum electrodynamics, provides a pathway to create and use large macroscopic quantum states with photons. Such states have been difficult to generate because atoms trapped in a cavity provide only weak nonlinearity to mediate photon-photon interactions, high photon loss introduces decoherence, low photon collection and detection efficiency decrease success probability, among other challenges. On the other hand, recent progress in superconducting qubits and high-quality microwave cavities for quantum computing has enabled orders of magnitude improvements in coherence, fast single shot high-fidelity readout, high-fidelity quantum operations, low photon loss, and better understanding of decoherence mechanisms. These advances have enabled early experiments that have demonstrated the creation of high-fidelity coherent states with several tens of photons. In addition, the new generation of superconducting devices opens up the opportunity for the exploration of new regimes of quantum optics involving quantum states of 100s of photons. Further advances are possible if, in addition to the physics of quantum optics, advanced microwave circuit engineering is brought to bear on the regime of low-power microwave signals to improve coherence and function, and materials science is employed to determine relationships between decoherence and defects in materials, surface chemistry, and interface quality. In turn, the superconducting systems and the quantum states created in them could also be used as sensitive probes of materials behavior, in particular of the origin and sources of decoherence and dissipation mechanisms.

The multidisciplinary research team led by Professor Houck combines the efforts of physicists and engineers who will develop the theoretical and experimental tools to establish new regimes of quantum optics using superconducting circuits. The new states of light established in this program provide new tools for metrology,

could provide key insight into non-equilibrium quantum systems, and in the long term may lead to applications in quantum communication and sensing.

10. Modular Quantum Systems. This MURI began in FY16 and was awarded to a team led by Professor Christopher Monroe at the University of Maryland – College Park. The goal of this research is to discover and explore modularity concepts for extensibility of small high-performance multi-qubit systems to larger systems with reduction of operational complexity. This research is co-managed by the Physics Division and AFOSR.

A paramount challenge in exploring physical systems (qubits) suitable for quantum information processing has been the contradictory requirement for precise manipulation of a quantum state on demand while maintaining strict isolation from the environment. Significant progress has been made in addressing this challenge. Coherence in several physical qubit types has improved by orders of magnitude. High fidelity fundamental quantum logic operations have been demonstrated. This progress has extended to multi-qubit systems involving a few (order ten) qubits. Progress continues to be made in improving coherence and fidelity. In parallel, advances have been made in connecting physically separated qubits. Key to these rapid advances has been a multi-disciplinary approach involving physics, materials science, control engineering, computer science, and mathematics, among other fields. A scientific challenge to further progress in the field has been the difficulty to add qubits and increase system size, while maintaining coherence and high-fidelity operations. System size needs to be increased before useful functionality can be explored and realized. Adding qubits increases the complexity of interactions between the qubits and makes layout, fabrication, and quantum control for high fidelity operations extremely challenging. Additional unwanted interactions introduce new qubit degrees of freedom to entangle with the environment and degrade coherence and fidelity. Modularity is a general scientific approach to address such complexity in which the system is decomposed into repeatable blocks with well-defined and controlled interfaces and interactions between the blocks and has been applied successfully to classical systems. Here, a module can be envisaged as a functional group of qubits and an interface. Exploring modularity for complex quantum systems is nascent but provides a potential extensible approach in which small numbers of high performance qubits can be extended to groups of high performance qubits and interfaces capable of precise manipulation within the group, between groups when required, and isolation from the environment and other groups.

Any quantum information processing system must balance the need for coherent control of the many interacting qubits necessary for a large-scale quantum system with decoherence rates that generally grow with system size. The objective of this research is to investigate a modular approach to constructing multi-qubit systems suitable for quantum information processing, to determine whether a modular system can achieve this balance and study the associated costs and benefits of taking the approach. In the long term, this research may overcome barriers and lead to new capabilities in the logistics, optimization, and the quantum simulation of materials.

11. Discovering Hidden Phases with Electromagnetic Excitation. This MURI began in FY16 and was awarded to a team led by Professor David Hsieh at the California Institute of Technology. The goal of this MURI is to discover and systematically explore hidden phases of materials induced with driven periodic excitation, to explore the unique physics and properties anticipated in those phases, and to illuminate the dynamics of the excitation process leading to them. This research is co-managed by the Physics (lead) and Materials Science Divisions.

Nascent research has demonstrated unique phases that are not adiabatically accessible from the known phase diagram. Recent discoveries have involved photo-excitation of a material with an ultra-short pulse which non-adiabatically induces a phase distinct from that existing elsewhere on the ground state phase diagram. Examples include a non-equilibrium superconducting state in a BCS superconductor, a ferromagnetic state in an antiferromagnetic oxide, and a unique metallic state in a thin film of a dichalcogenide. Also of interest are novel phases that can be adiabatically driven via a continuous periodic excitation (a.k.a. Floquet) that drives a material into a new phase (e.g. inducing a topological surface state in an ordinary insulator.) The additional time-periodic potential adds a new term to the Hamiltonian and drives, for example, transitions in orbital ordering, new electronic states with new crossings and avoided crossings, and resonant enhancement or reduction of superconducting order or charge and spin density waves.

Much opportunity is provided by recent advances in THz sources with MV/cm level electric fields which are sufficiently strong to provide resonant excitation of order parameters in strongly correlated materials. Additional opportunities are presented by van der Waals layered materials and free standing materials with reduced

connections to the environment, thus limiting sources of decoherence. The objective of this research is to design, realize and manipulate new phases of matter using electromagnetic excitation, that in the long term may lead to enhancements of electronic, optical, magnetic and thermal material properties that would lay a foundation for future technology in many areas.

C. Small Business Innovation Research (SBIR) – New Starts

The Division did not have any new-start SBIR contracts in FY16; however, the Division managed active projects continuing from prior years. A list of SBIR topics published in FY16 and a list of prior-year topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY16, the Division managed two new-start STTR contracts, in addition to active projects continuing from prior years. These contracts aim to bridge fundamental discoveries with potential applications. A list of STTR topics published in FY16 and a list of prior-year topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY16, the Division managed one new ARO (Core) HBCU/MI project and three new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The following PECASE recipient, previously nominated by this Division, was announced in this fiscal year by the White House. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Coupled Synthesis, Transport, and Magnetization Studies to Detect Topological Phases. The objective of this PECASE, led by Professor James Rondinelli at Northwestern University, is to pursue the rational design of quantum many-body phenomena by engineering artificially layered oxides.

In particular, this research aims to design non-centrosymmetric complex oxides metals from first principles and achieve noncentrosymmetric oxides that are conducting at room temperature and at fixed stoichiometry, by interleaving bulk perovskite TMOs together into heterostructure and superlattice geometries. If this research is successful, it may ultimately lead to remotely interrogated passive sensors, electro-optic modulators at THz frequencies, ultra-sensitive detectors and ultra-low power electronics.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY16, the Division managed five new DURIP projects, totaling $1.4 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. Joint Technology Office - High Energy Lasers (JTO-HEL)

The JTO-HEL program is designed to model, fabricate, and characterize rare-earth (RE) doped, single-crystal (SC) fibers for the use as high power lasers and amplifiers. The basic concept behind this research program is to take advantage of the high power capability of RE-doped oxide crystals to fabricate SC fibers that have the potential of exceeding the output of glass fiber lasers used today. Future plans include further cladding studies of SC fibers, further index profiling, and pumping the doped YAG fibers to achieve higher laser power in the wavelength range between 1600 to 2100 nm. This program is co-managed by the Physics and Electronics Divisions.

I.   DARPA Quantum Assisted Sensing and Readout (QuASAR) Program

The goal of this program, co-managed by the Physics Division, is to bring state-of-the-art science of metrology and sensing and combine them with today's technological developments. The program goal is to bridge the gap between the best scientific performance and the appropriate packaging for fielding high-performance working sensors that are relevant to the DoD. This program was motivated in large part by the Physics Division and compliments ARO-supported research in ultracold gases, providing theoretical and experimental synergy to the Core program.

J.   DARPA - Fundamental Limits of Photon Detection (Detect) Program

The Detect program seeks to establish the first-principles limit of photon detector performance. Currently, the performance of different classes of photon detectors varies significantly with respect to key metrics and fundamental limits of performance are not fully understood. Detect aims to establish these fundamental limits by developing new models for a variety of technology platforms and testing those models in proof-of-concept experiments. The program, co-managed by the Physics Division, is exploring whether new approaches could achieve the best performance characteristics from all current detection platforms and exceed current performance in all metrics simultaneously. The scope of this research effort is extremely well matched with efforts in the QIS program and work previously funded by ARO in single photon detection, a critical aspect of several quantum information processing approaches.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Physics Division.

A. Exploring Strong Coupling Between Quantum Dots and Nanocavities
Professor Jelena Vuckovic, Stanford University, Single Investigator Award

Quantum dots (QDs) are appealing candidates for quantum bits because of their optical addressability, narrow linewidths, and ease of integration into optoelectronic devices. To explore their potential, however, QDs must be controlled in a way which does not inhibit these properties. Strongly coupling a dot to a nanocavity is a potential path to this goal, but to date dissipation has hindered the complete coherent control of QD-cavity systems. In FY16, however, Professor Vuckovic and her team devised a scheme to achieve this control in a strongly coupled QD-photonic crystal cavity experiment. By carefully detuning the resonances of the QD and the cavity the team was able to isolate the energy levels of interest of the polaritons created by the hybridization of the electromagnetic waves and matter in the system. This, in turn, allowed for a compromise between the spectral width of the excitation laser and the necessary short pulse lengths required for single excitations. This novel approach along with a minimization of the leakage of noise into the detection path enabled the team to observe Rabi oscillations in their system, a fundamental signature of a coherent interaction between their excitation laser and the polaritons (see FIGURE 1). The group then varied the laser excitation power in a two pulse experiment to rotate the Bloch vector of the polariton to a superposition of ground and excited states, and varied the phase difference between the pulses to successfully rotate the Bloch vector across sphere. This achievement means that complete coherent control of the system was successfully demonstrated, thereby opening the door to making strongly coupled QD-photonic crystal cavity systems viable candidates for quantum on-chip photonic devices.
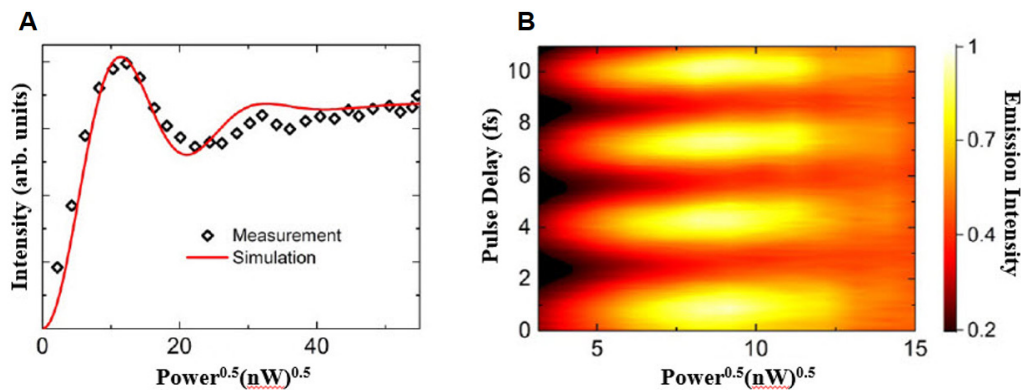

FIGURE 1

Coherent control of a quantum dot strongly coupled to a nanocavity. (**A**) The observed Rabi oscillations for a resonant excitation of a polariton state are shown in part. The oscillations are a fundamental signature of the coherent interaction between the polaritons and the excitation laser pulses. The red line in the plot shows a simulation run in order to better understand damping in the system, and the results indicate that dephasing originating from phonons and excitation pulses are the primary causes. (**B**) Data illustrating complete coherent control of the strongly coupled QD-photonic crystal cavity system. Both the excitation power and phase difference were swept in order to establish that any point on the Bloch sphere can be reached by the system, thereby showing that the team truly achieved complete coherent control.

B. Coherence Times of Bose-Einstein Condensates beyond the Shot-Noise Limit via Superfluid Shielding
Professor Wolfgang Ketterle, Massachusetts Institute of Technology, MURI Award

Applications such as quantum information, quantum metrology, atom interferometry, and force sensing derive their high precision by exploiting quantum mechanics, specifically by measuring the phase coherence between spatially separated quantum objects. There are fundamental limits to how well an object can be prepared,

operated upon and have the phase relationship read out via interference. In addition to these fundamental limits, the performance of these quantum systems can be limited by technical and environmental noise that results in reducing coherence time. For this reason most applications have relied on non-interacting systems because the final precision in the measurement of the phase is determined by the classical shot noise.

In 2016 ARO funded researchers demonstrated a new method of enhancing the phase coherence time of spatially separated Bose Einstein Condensates (BECs) beyond the shot-noise limit by immersing the system in a superfluid bath, a method the researcher's referred to as "superfluid shielding." The superfluid bath shields the separated BECs from phase fluctuations associated with both density dependent self-interactions and external environmental forces. The density distribution of the superfluid bath is free to modify itself, which results in the cancelation of both sources of phase fluctuations and preserves the coherence of the spatially separated BECs.

To experimentally demonstrate that this new strategy can greatly extend the relative phase coherence of spatially separated BECs, ARO-funded researchers monitored Bloch oscillations of two spatially separated BECs in an optical lattice. In an optical lattice, the phase coherence and number fluctuations of a BEC can be probed by a sudden application of a large acceleration to the lattice which leads to the phenomenon of Bloch oscillations, which was used to create separated condensates and probe their phase coherence. The researchers found that when unshielded, the cloud is diffuse which is indicative of decoherence (see FIGURE 2). However, in the superfluid shielding cased both high contrast and Bloch oscillations are present indicating phase fluctuations have been dampened by the bath. Theoretical analysis published in *Physical Review Letters* 117, 275301 shows that fluctuations in the chemical potential can be reduced by up to two orders of magnitude for ^{87}Rb condensates using this method.
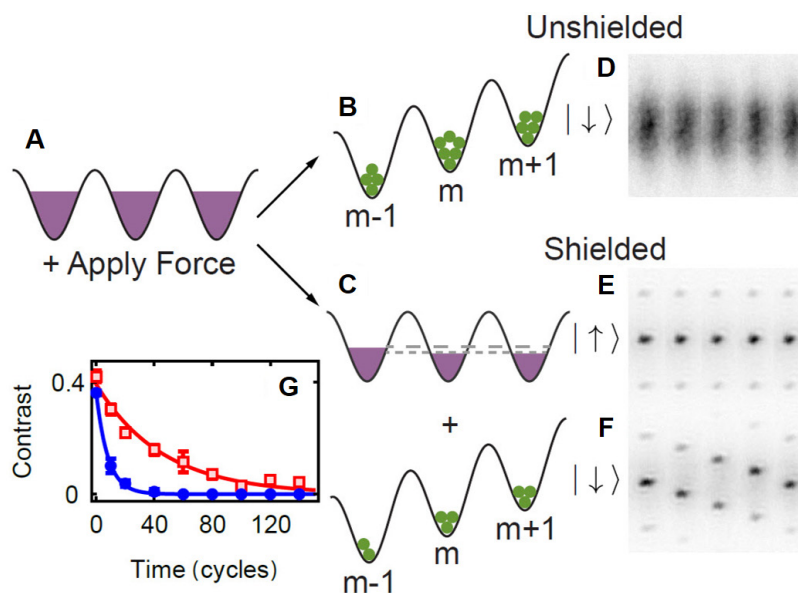

FIGURE 2

Schematic of superfluid shielding. (A) Before applying a tilt, the atoms are in a superfluid, which is approximately described by a coherent state on each site. The chemical potential is constant across the cloud. (B) In the limit of a strong tilt ($\Delta \gg J$), the wave function at each lattice site is projected onto the number basis, leading to fluctuations in the number of atoms and chemical potential from site to site. (C) If the gas has two components, one which is localized by the tilt, and one which remains superfluid, the itinerant component can compensate for fluctuations in the localized component. (D)-(F) Momentum distribution over the course of a single Bloch oscillation after ten cycles. (D) Without superfluid shielding, the diffuse cloud indicates decoherence of the condensate. (E) The itinerant component feels no force and does not Bloch oscillate. (F) For the shielded component, the Bloch oscillation contrast is high. (G) Exponential decay of the Bloch oscillation contrast for a one-component (blue dots) and two-component (red squares) gas, for a transverse lattice depth of 11 Er and ~8 x 10 3 atoms.

Progress in atom interferometry using BEC has been limited due to decoherence associated with density fluctuation and environmental noise. ARO-funded researchers have developed and demonstrated a new strategy that uses a superfluid bath to shield the condensates from the two leading sources that limits coherence and

therefore performance. This breakthrough in "superfluid shielding" may contribute to further advances in quantum computing and precision navigation.

C. Novel Microwave Based Ion Trap Entanglement Architectures For Quantum Computation
Professor Winfried Hensinger, University of Sussex, Single Investigator Award

Trapped ion qubits are promising candidates for use in quantum computation systems capable of beyond classical functionality. In state-of-the-art designs, however, the number of required lasers scales with the number of ion qubits and this quickly makes many-qubit experiments intractable. Long-wavelength radiation coupled with static magnetic field gradients can be used as alternatives to 100% laser based schemes but, to date, this approach also suffers from scaling difficulties.

In FY16 Professor Hensinger and his group attacked this tractability problem with a novel approach. They utilize global long wavelength radiation fields in conjunction with static magnetic field gradients, but integral to the scheme is the requirement of ion qubits that feature a widely tunable transition frequency robust to ambient magnetic field fluctuations. Clock qubits utilizing "dressed states" meet this requirement and the group chose to use two $^{171}Yb^+$ ions prepared as clock qubits to demonstrate key elements of their approach (see FIGURE 3). During the experiment, the "clock like" qubit was created and, in contrast to standard clock transitions with a fixed energy splitting, the qubit's transition frequency is tunable via magnetic fields. This tunability is crucial for the ultimate scaling of the system. After qubit preparation, a maximally entangled state was created using a Molmer-Sorensen type gate and the coherence determined. The data indicate the system has a Bell state fidelity of 0.985, which places it among the best two qubit gate fidelities achieved. Going forward, the group will work to improve their fidelity and move to a scheme where locally applied currents supply magnetic field gradients on demand. This will ultimately enable the control of individual transition frequencies of clock qubits in and out of resonance with global radiation fields. This provides a potential pathway toward a scalable architecture where each logic gate location is individually controlled analogous to the way traditional transistors are controlled within classical computer architectures.
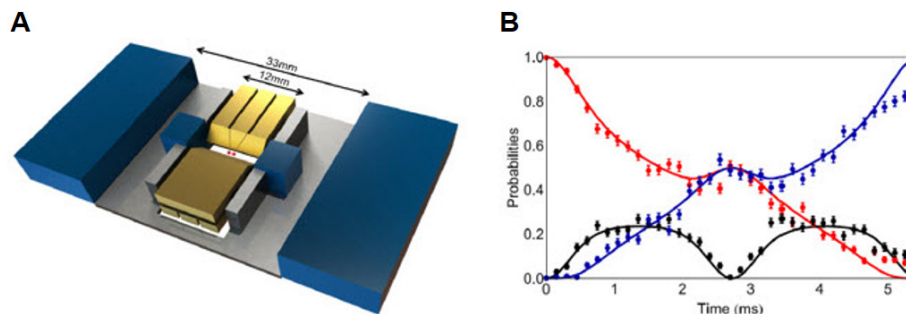

FIGURE 3

Ion trap quantum computing architectures with global radiation fields. (**A**) Schematic of the experimental setup, showing the linear ion trap (yellow) fitted with four permanent magnets (blue), arranged to create a strong magnetic field gradient along the trap axis. Representative ions are shown in red, not to scale. After the system is prepared, a Molmer-Sorensen two-qubit gate is applied for a variable amount of time, t, utilizing long-wavelength radiation and the static magnetic field gradient. (**B**) Probability of the (up, up) state in red, (down, down) in blue, and (up, down) + (down, up) in black as a function of applied gate time. The plot shows a maximally entangled state is formed at time t = 2.7 ms. Further measurements to extract the coherence of the system indicate a Bell state fidelity of 0.985(12), which is among the best two-qubit gate fidelities achieved.

D. Intrinsic Coupling Of Magnetism With Topologically Non-Trivial States
Professor J. Checkelsky, Massachusetts Institute of Technology, Single Investigator Award

With the scientific importance of topologically non-trivial electronic states in the solid state having been well established, there is a concerted effort to explore the interplay between topology and strong correlations. Magnetism and superconductivity have fared prominently as correlated phenomena of interest in this effort with success in both. For example, topological insulators doped with magnetic atoms have been shown to exhibit a quantum anomalous Hall effect – quantized conductance without a magnetic field present. Superconductivity

has also been induced by proximity in topological insulators and topological semimetals with unusual phenomena resulting.

This research involves a more challenging situation in which magnetic order and topological state coexist intrinsically. GdPtBi, a part of the half-Heusler family of materials, is a promising candidate for such coexistence. It is comprised of interpenetrating face-centered cubic lattices; one for each element. The Gd sub-lattice organizes itself into an antiferromagnet with each layer along the cube's trigonal axis having spins pointing in the opposite direction. The Pt and Bi sub-lattices work together to form electron energy levels at the chemical potential. They are heavy elements with large spin-orbit coupling and exhibit phenomena akin to topologically non-trivial effects. The characteristic that reveals the uniqueness of this material is an anomalous Hall effect. The ratio of the transverse to longitudinal conductivity far exceeds that have been observed in other antiferromagnets, and is comparable to ferromagnets (see FIGURE 4). This points to unique mechanism for the Hall effect – the intrinsic band structure. While the precise nature of the band structure topology of GdPtBi is not known, this anomalous Hall effect reveals a significant Berry curvature which is tightly coupled to topologically non-trivial band structure. Mathematically, the Berry curvature is equivalent to a magnetic field in the electrons' momentum space. As electrons travel through the crystal, changing momentum, the wavefunction picks up a phase shift resulting from this curvature. For topologically non-trivial materials, this phase shift is not a multiple of 2π when it comes full circle in momentum space, causing, among other things, a Hall effect.

This initiative is revealing that heavy elements in which f-electrons and 5d-electrons are present are a likely source of unique phenomena for new scientific discoveries. Concurrently, this particular study, while showing effects only at temperatures of a few kelvin, suggests that materials which combine topologically non-trivial effects with magnetism may revitalize the potential of low power consuming spintronic applications.
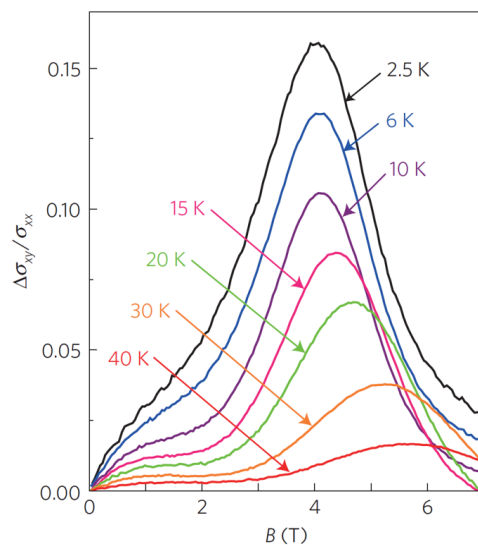

FIGURE 4

The anomalous Hall effect in GdPtBi. At the lowest temperature measured, 2.5K, the ratio of transverse to longitudinal conductivity (y-axis) exceeds 0.15. This is roughly an order of magnitude larger than observed for any other antiferromagnet known to date.

E. Parity-Time Photonic Synthetic Media: From Nonlinear and Singular Optics to Lasing
Professors Liang Feng (lead PI) and Natalia Litchinitser (co-PI), State University of New York - Buffalo, Single Investigator Award

The objective of this research is to investigate novel photonic media based on the synergy of two emerging fields of parity-time symmetry and structured light in both linear and nonlinear regimes. The first year of this research led to the first experimental demonstration of orbital angular momentum (OAM) microlasing action through the novel photonic cavity tailored at an exceptional point (see FIGURE 5). The structured microlasing radiation was obtained by structuring the photonic media in a parity-time symmetric fashion.
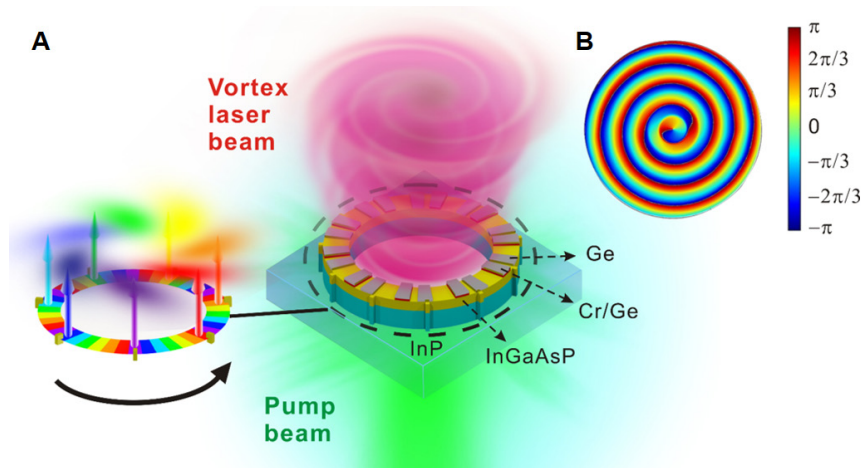
FIGURE 5

OAM Microlaser emits the vortex laser beam. (A) Schematic of the OAM microlaser, where combined complex-index modulations are introduced through Ge and Cr/Ge layers on top of the micro-ring. (B) Simulated phase distribution of laser radiation, presenting a charge-1 vortex with a topological phase singularity point at the beam axis.[5]

A conventional micro-ring cavity supports whispering gallery modes circulating inside the cavity in both, clockwise and counter-clockwise directions. While each of these modes carries OAM, these OAMs cancel each other when the two counter propagating modes are simultaneously excited. Therefore, in order to produce a laser beam carrying an OAM in such a cavity, a unidirectional power circulation is required. In their work, they introduced a carefully designed complex refractive index modulations on the top surface of the micro-ring laser that allows the selection of either clock-wise or counter-clockwise circulating mode. Furthermore, they added sidewall modulations periodically arranged along the micro-ring outer walls in order to extract the OAM mode upwards into free space. The single-mode microlaser was fabricated on the III-V semiconductor platform and experimentally verified through self-interference measurements (see FIGURE 6). This microlaser was the first independent micro/nanoscale laser sources emitting complex vector beams carrying the OAM information available for an ultimate miniaturized optical communication platform. Recently, the PI's discovery was highlighted in the 2016 *OSA Optics and Photonics News*.[6] The demonstration on the OAM microlaser is expected, in the long term, to improve the speed and throughput of data transmission and storage methods.
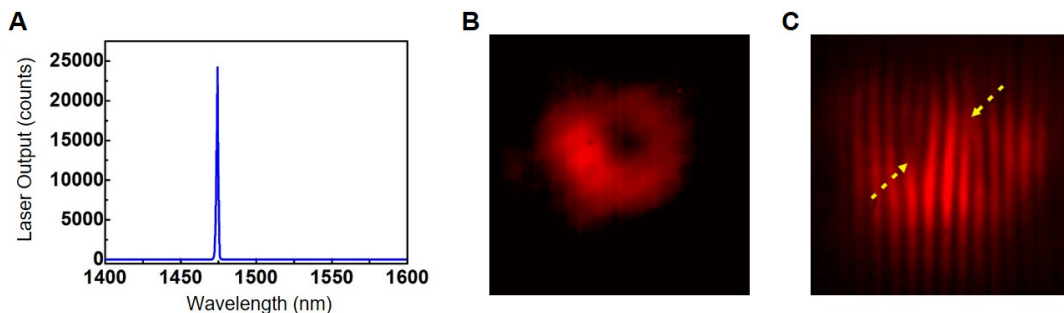

FIGURE 6

Characterization of OAM lasing. (A) Laser emission spectrum. (B) Far field intensity distribution of the laser emission. (C) Off-center self-interference of the OAM lasing radiation, showing two inverted forks (marked with arrows) and validating the OAM charge.[5]

[5] Miao P, Zhang Z, Sun J, Walasik W, Longhi S, Litchinitser NM, Feng L. (2016). Orbital angular momentum microlaser. *Science*. 353: 464-467.

[6] Miao P, Zhang Z, Sun J, Walasik W, Longhi S, Litchinitser NM, Feng L, (2016). Orbital angular momentum microlaser. *OSA Optics and Photonics News*. 32.

F. Spatially resolved studies of the insulator-to-metal phase transition in V_2O_3
Professor Dimitri Basov, University of California San Diego, Single Investigator Award

Vanadates are prototypical correlated oxides with Mott insulator-to-metal transitions that occur between 150K and 350 K, depending on the stoichiometry. They are studied extensively as playgrounds in which to observe correlated electron phenomena and have also found broad application ranging from catalysis to bolometry. However, the nature of the renowned phase transition is poorly understood and itself is a subject of much study. In FY16, Professor Basov published a specialized technique to reveal the phase transition of one of the well-known vanadium oxides in great detail.[7] Of primary interest is whether the transition is electronic in nature and drives a structural transition or if the transition is structural in nature driving a different electronic structure.

The technique used involves a scanning probe as a near-field antenna to couple infrared light to the nanometer scale. Light from an infrared laser impinging on an atomic force microscope (AFM) tip couples the infrared light to the surface of a sample. The scattered light is detected and the optical response of the material is measured with a spatial resolution of roughly 10 nm. Conveniently, the use of an AFM tip provides the opportunity to also study the material with various other modalities available with AFM arrangements such as physical topology and magnetic order. Professor Basov has employed this technique to study the V_2O_3 phase transition. By precisely controlling the temperature of the sample during measurement, he is able to arrest the thermally induced phase transition mid-course and study various local characteristics of the material (See FIGURE 7).
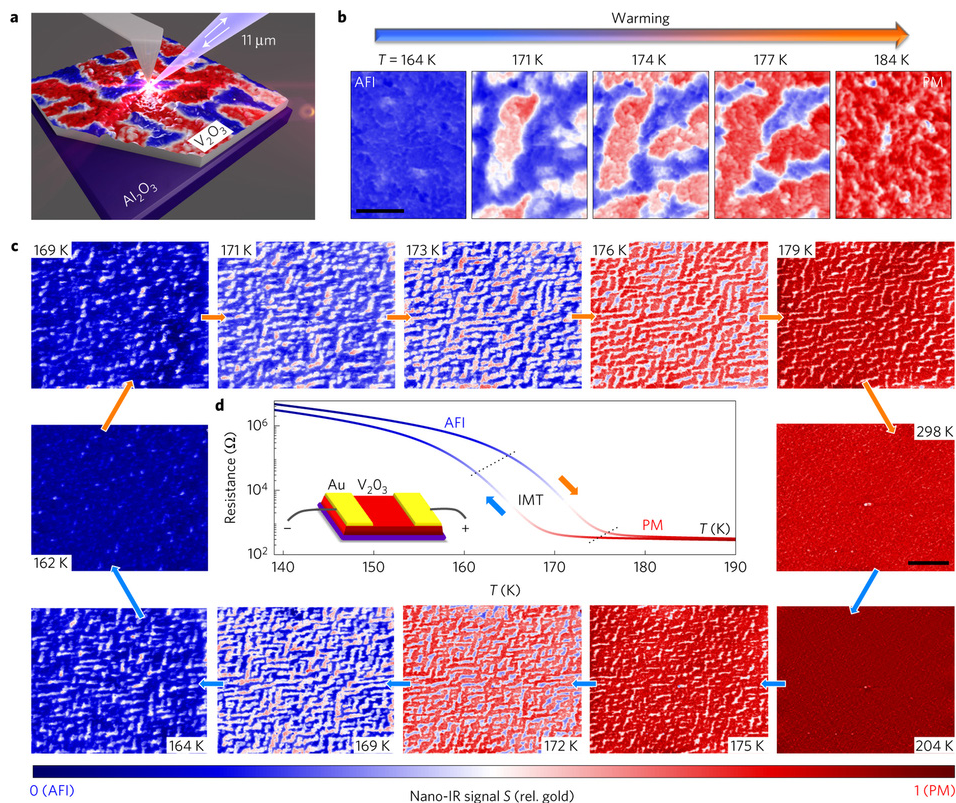

FIGURE 7

Watching the V_2O_3 metal-insulator phase transition. Metallic regions are red and insulating regions blue. The top panel shows a schematic of the technique and high resolution detail of the transition going from cold (insulating) to warm (metallic). Scale bar is one micron. The lower panel shows the full temperature cycle around the hysteretic resistance-vs-temperature plot in the center. Scale bar (far right) is five microns.[7]

This study provides direct information about a number of aspects of the phase transition that were previously only theoretically expected. First, it is clear that this is a first-order phase transition with percolating puddles of

[7] McLeod AS, van Heumen E, Ramirez JG, Wang S, Saerbeck T, Guenon S, Goldflam M, Anderegg L, Kelly P, Mueller A, Liu MK, Schuller IK, Basov DN. (2017). Nanotextured phase coexistence in the correlated insulator V_2O_3. *Nature Physics*. 13:80-86.

one phase within the other. The most unique result of this study is the comparison with x-ray diffraction data. Insulating V_2O_3 has a monoclinic crystal structure whereas metallic V_2O_3 has a corundum structure. However, during the transition, the percentage of metallic regions significantly exceeds that of the corundum regions: the electronic phase bleeds into the monoclinic structure otherwise known for its insulating character (see FIGURE 8) This reveals that the electronic phase transition and the structural phase transition are to some degree decoupled.
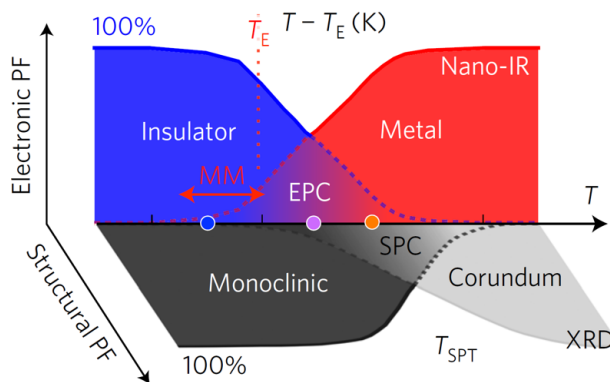

FIGURE 8

Comparison of electronic and structural phase transitions. Note how the transition regions of the two are offset from each other (PF = phase transition; EPC = electronic phase change; SPC = structural phase change).[7]

While the precise origin of this decoupling is yet to be determined, length scale of the metallic islands, their striped nature, and several theoretical studies suggest that Coulomb interactions are involved. However, the additional insight from this study provides new opportunities to understand the details of insulator-metal phase transitions. The technique is being applied to other phase change materials and will certainly play a significant role in elucidating a complete model of phase changes in the solid state.

G. New Regimes in Quantum Optics with Superconducting Circuits
Professor Andrew Houck, Princeton University, MURI Award

Improvements in superconducting quantum systems over the past decade have enabled their use in the exploration of entirely new regimes of physics, including the emergence of matter-like properties of light in many-body quantum optics experiments. In particular, superconducting circuit quantum electrodynamic (QED) systems are now well suited for studying non-equilibrium phase transitions. The ease with which photons can be added to these systems enables the balance of drive and dissipation, and correspondingly makes the study of previously intractable non-equilibrium problems accessible.

In FY16, the MURI team lead by Professor Andrew Houck explored a non-equilibrium steady state circuit QED system with the goal of observing a dissipative phase transition, a transition in which the steady state, rather than the ground state, abruptly changes as a parameter is varied. The experiment utilized a one-dimensional chain of 72 microwave cavities each strongly coupled to a superconducting qubit (see FIGURE 9). The team balanced drive and dissipation to achieve the non-equilibrium steady state and then measured transmission through the chain as a function of drive frequency and power (photon number). At low power, transmission peaks emerged consistent with small interaction-induced shifts caused by the qubits. At higher power, however, a marked change in the transmission emerged and the peaks split to give rise to a region of low transmission. The low to high power transition is hysteretic, depending on the direction that the power is swept, and bistable, switching stochastically between two states. Further study of the switching revealed an asymptotic decay rate nearly five orders of magnitude slower than other decay rates in the system. This exceptionally long switching time is characteristic of a dissipative phase transition, as is the observed loss of all resonance peaks at higher drive powers. This experiment demonstrates the power of circuit QED systems for studying non-equilibrium condensed matter physics and paves the way for future experiments exploring non-equilibrium physics with many-body quantum optics.
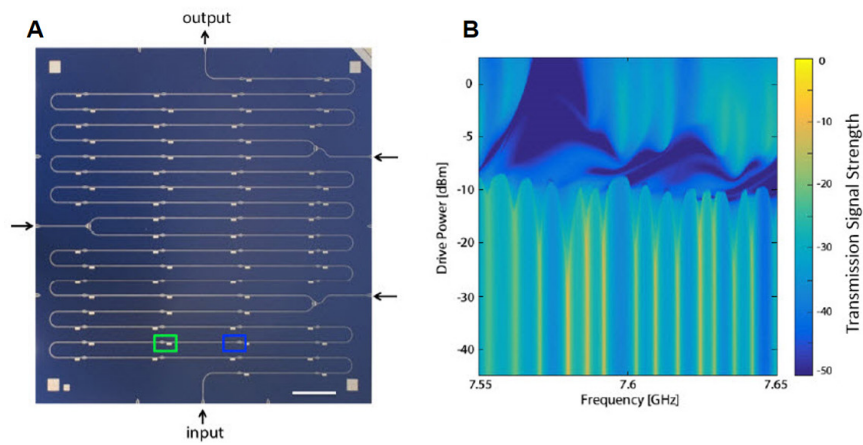
FIGURE 9

Phase transitions in circuit quantum electrodynamic (QED) systems. (A) 72-site circuit QED lattice utilized in the dissipative phase transition experiment. The green box highlights one of the 72 qubit-microwave resonator locations. (B) Microwave transmission spectra from the chain of microwave cavities as a function of driving power (number of photons in the system) and frequency. The abrupt transition to a suppressed transmission regime at high driving power and split into a region of bistability is indicative of a dissipative phase transition.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Novel Process Development for On Chip High Magnetic Field Ion Traps
Investigator: Professor Winfried Hensinger, University of Sussex, Single Investigator Award
Recipient: ARL-SEDD

The goal of this research is to develop methods to perform high-fidelity quantum logic and quantum control experiments with trapped ions using microwaves in microfabricated ion trap chips. This objective is in contrast to many trapped ion experimental efforts which rely on lasers for manipulation of the ions, but will potentially result in ion trap experiments which are much easier to scale up than their laser based counterparts. Correspondingly, this effort relies heavily on innovative chip designs. One such design incorporates embedded current-carrying wires to provide the extreme magnetic field gradients necessary to execute the proposed scheme. The fabrication process for the embedded wires is highly experimental and its development is a crucial component of Professor Hensinger's work.

This research has transitioned to ARL-SEDD, where Professor Hensinger's team and ARL researchers will collaborate in the fabrication of novel ion trap chips. To date, the efforts at ARL-SEDD have produced chips capable of applying 10 A of current in continuous operation. The magnetic field gradients which correspond to this current should be enough to realize quantum gate times of 50 microseconds and fidelities in excess of 99%. The development work between the teams is currently ongoing and it is ultimately hoped that ARL's cleanroom facilities can be leveraged to research and fabricate traps which will facilitate scalable, multiqubit experiments.

B. Quantum Cascade Laser-based Portable Spectrometers
Investigator: Professor Federico Capasso, Harvard University, Single Investigator Award
Recipient: Pendar Technologies, LLC

Professor Capasso's research to develop quantum cascade lasers (QCLs) was funded in part through ARO in the late 1990s and early 2000s. In addition, ARO co-managed DARPA program support for Professor Capasso's research to extend QCL capability to mid- and far-infrared wavelengths and to higher operating temperatures. These results transitioned to EOS Photonics in 2010 to develop marketable technology based on the QCL. In FY16, EOS Photonics merged with Pendar Medical to form Pendar Technologies, LLC which is developing portable spectroscopy and chemical sensing products based in part on QCL technology.

V.   ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Chip-Based Optical Parametric Oscillators for Coherent Computing and Quantum Random Number Generation
Professor Alexander Gaeta, Columbia University, Single Investigator Award

Combinatorial optimization problems are becoming ever more important to society and will impact many future DoD capabilities, specifically autonomous systems. Optimization problems found in cognitive networks, artificial intelligence, and the analysis of social networks are examples where problems classified as non-deterministic polynomial time (NP)-hard or NP-complete problems are encountered and are considered intractable with modern computers. It is known that many combinatorial optimization problems can be mapped onto the ground-state search problems of the Ising Hamiltonian. There is recent evidence that degenerate optical parametric oscillators can be used to form a large-scale network of artificial spins providing an experimental Ising machine capable of solving difficult optimization problems. A recent report in a non chip-based system demonstrated a network of >10,00 spins bringing this computational paradigm very close to solving real world problems.[8]

It is anticipated that in FY17, Professor Gaeta will experimentally realize a chip-based spin system in silicon, which should reduce size and power while maintaining computational efficiency. If he is successful demonstrating this new computational systems, it may provide a new computational paradigms that may provide critical solutions to the technical challenges that DoD anticipates facing in its pursuit of autonomous systems and network optimization.

B. Topologically Protected States of Light
Professor Andrew Houck, Princeton University, MURI Award

One objective of this research is to elucidate how to build topological materials with microwave photons. While it is known that microwave photons are ideally suited to quantum optics experiments, realizing the non-reciprocity in the systems necessary to explore topological physics has remained elusive. Non-reciprocal one-way elements would open up entirely new directions for exploration in superconducting cavity systems including the realization of topologically protected transport of excitations and the emergence of fractional quasi-particles due to many-body interactions. Year one of the MURI was enormously successful in laying the groundwork for the exploration of this type of physics. The group used established techniques from cavity and circuit quantum electrodynamics to develop a scalable architecture for the exploration of interacting topological phases of photons in arrays of microwave cavities and incorporated a time-reversal symmetry breaking (non-reciprocal) flux in their system via a coupling between the microwave cavities and ferrites. The group leveraged these successes to build a metamaterial which can realize a Chern insulator, and this metamaterial will be a point of focus in the year to come.

It is anticipated that in FY17, the MURI team will fully characterize their room temperature version of the microwave Chern insulator, and in particular study its time domain propagation fields with single lattice site resolution. If successful, this could enable the first-ever real space measurement to directly measure the Chern number of each band of the system.

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[8] Inagaki T, Inaba K, Hamerly R, Inoue K, Yamamoto Y, Takesue H. (2016). Large-scale Ising spin network based on degenerate optical parametric oscillators. *Nature Photonics*. 10: 415-419.

C. Non-centrosymmetric Polar Metals
Professor James Rondinelli, Northwestern University, PECASE and Young Investigator Program Award

Materials exhibiting metallic behavior almost invariably preserve inversion symmetry. The free electrons screen out the long-range electrostatic forces that cause atomic displacements. In insulating ionic materials, such displacements minimize the crystal's free energy and result in polar (i.e. ferroelectric) order. However, counter examples do exist. The objective of this research, led by Professor Rondinelli, is to elucidate the microscopic origins in which inversion-symmetry breaking can co-exist with metallicity and develop reliable crystal-chemistry guidelines to encourage future discoveries and the direct engineering of polar metals. Professor Rondinelli has made significant progress in this area to date. It is anticipated that in FY17, he will have data demonstrating these interesting phases. Such materials would enable the unusual combination of metallic properties with optically active properties.

D. Flat Photonics with Metasurfaces
Professor Vladimir Shalaev, Purdue University, Single Investigator Award

A meta-surface is a new type of 2D metamaterial inheriting all the merits held by metamaterials (MMs). Recent progress in meta-surfaces could address major issues—such as high loss, cost, ineffective fabrication, and challenging integration that are hampering the further development of MM technology. This progress could result in the development of new types of ultrathin meta-surfaces with unparalleled properties including increased operational bandwidths and reduced losses. It is anticipated that in FY17, the ARO-funded research team will achieve real time dynamic control by using an external beam or field to change the properties of the meta-surface. This development could lead to novel, ultrathin devices that offer unprecedented functionalities including dynamic spatial light modulation, pulse shaping, beam steering, novel quantum optics devices, and nanoscale resolution imaging and sensing.

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