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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 2014 (FY14; 1 Oct 2013 through 30 Sep 2014). 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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2014
ARO
IN REVIEW

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U.S. Army Research Office (ARO)
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ARO IN REVIEW 2014

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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 Laboratory's Army Research Office (ARO) for fiscal year 2014 (FY14; 1 Oct 2013 through 30 Sep 2014). 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 these disciplines: chemical sciences, computing sciences, electronics, life sciences, 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 also ensures 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*.

The ARO strategy and programs are formulated in consultation with the ARL Directorates, 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 DoD Quadrennial Defense Review (QDR), the DoD Strategic Basic Research Plan, the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)] S&T Priorities, the Army Science and Technology (S&T) Master Plan, the Army S&T Challenge Areas, the Training and Doctrine Command (TRADOC) Army Capabilities Integration Center's Integrated S&T Lines of Effort, the Assistant Secretary of the Army for Acquisition, Logistics, and Technology

[ASA(ALT)] Special Focus Areas, and the ASA(ALT) Triennial Basic Research Review. In addition, ARO's parent organization, the Army Research Laboratory, has eight Science and Technology Campaigns, including an extramural basic research campaign that ARO leads. For the other seven campaigns, which include research from Human Sciences to Materials, ARO supports research that will increase our fundamental knowledge and understanding of the physical, engineering, and information sciences as they related to long-term national security needs and the ARL Campaigns. 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 the science and technology (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 initiatives. 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). The National Defense Science and Engineering Graduate (NDSEG) fellowship program is one 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 an ongoing and active collaboration with a variety of Federal research organizations, including the:

- 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)
- Research, Development, and Engineering Centers (RDECs) within the Research, Development and Engineering Command (RDECOM)
- Army Medical Research and Materiel Command (MRMC)
- Army Corps of Engineers
- Army Research Institute for the Behavioral and Social Sciences
- Army Training and Doctrine Command

ARO's extramural research program provides foundational discoveries in support of the ARL S&T Campaign Plans. 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 the Army Corps of Engineers, 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 university center.

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. Other members of this group include the Assistant Secretary of Defense for Research and Engineering ASD(R&E) and representatives from the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR) and the Defense Advanced Research Projects Agency (DARPA).

IV. REVIEW AND EVALUATION

ARO Directorates, Divisions, and Programs are evaluated by a wide range of internal (Army) and external (Academic, other Government) reviews. Examples include the triennial Army Basic Research Review and 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).

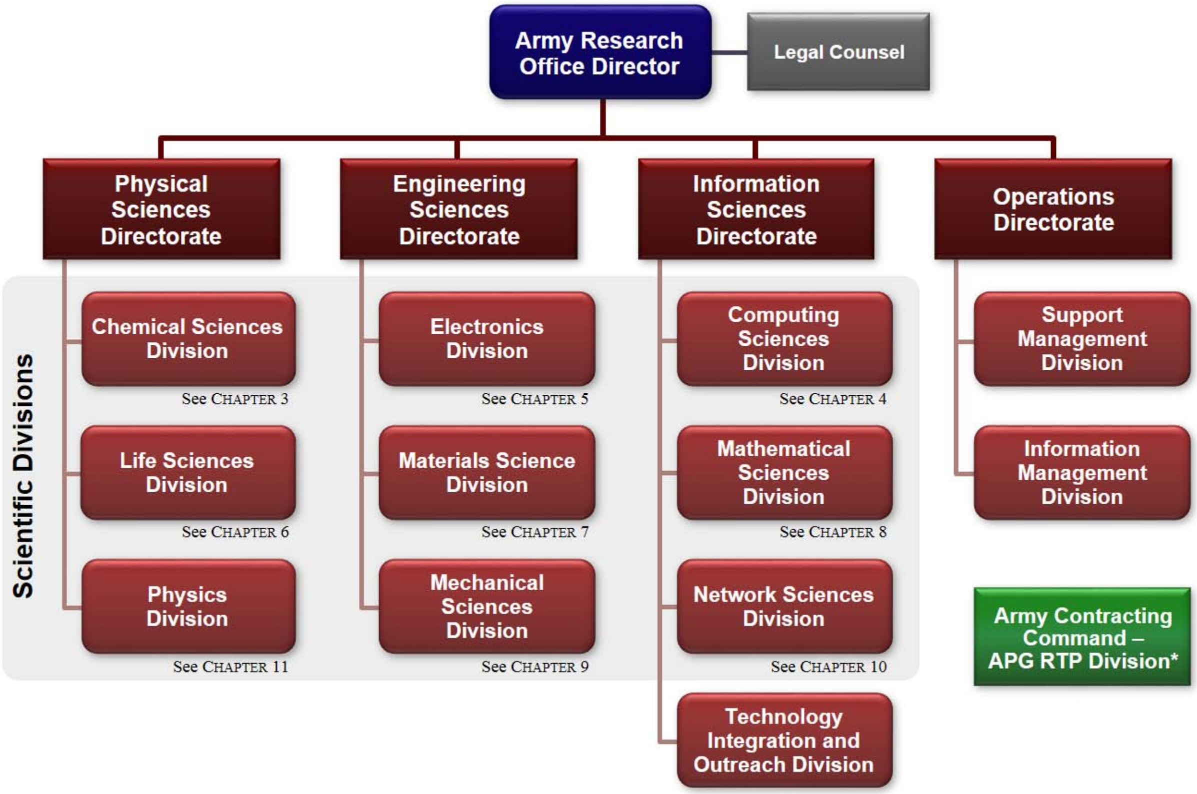

FIGURE 1

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. Note that the former Environmental Sciences Division and its programs began a reorganization process in FY14, to be completed in FY15. *The 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, it also performs contracting activities throughout RDECOM.

VI. ARO DIRECTOR'S OFFICE STAFF

Dr. David Skatrud
ARO Director
ARL Deputy Director for Basic Science

Dr. Stephen Lee
Chief Scientist

COL Thomas Ryan
Military Deputy

Mr. Edward Beauchamp, Esq.
Legal Counsel

Mr. Richard Freed
Associate Director for Business and Research Administration

Dr. Brian Ashford
Special Assistant to the Director

Ms. Marie Sander
Secretary to the Director

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 these disciplines: chemical sciences, computing sciences, electronics, life sciences, materials science, mathematical sciences, mechanical sciences, network sciences, and physics. ARO implements these 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 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 discussed in the following subsections.

A. Army Funding

The Army funds the majority of the extramural basic research programs managed by ARO. These programs are indicated below and are described in more detail later in this chapter.

- 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 Institutions (HBCU/MI; 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/MI 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 opportunities, 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-B.

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/MI 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).

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 mutidisciplinary 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.

Management 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 manage the MURI projects. The OXRs include ARO, the Air force Office of Scientific Research (AFOSR), and the Office of Naval Research (ONR). OXR program managers 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 FY14. These projects are based on proposals submitted to the FY14 MURI topic BAA, which was released in late FY13. The new-start projects, lead investigators, and lead performing organizations are listed below. The corresponding MURI topic, topic authors / program managers, and the ARO Division responsible for monitoring the projects are listed in parentheses. A description of each of these projects can be found in the corresponding Division's chapter.

- Mechanisms of Force Sensing in Adherent Cells as Inspiration For New Materials; Professor Margaret Gardel, University of Chicago

  (Topic: *Force-Activated Synthetic Biology*; Dr. Stephanie McElhinny, Life Sciences, and Dr. David Stepp, Materials Science)

- Understanding the Skin Microbiome through the Integration of Metagenomics, Bioinformatics, Spatial Ecology, and Synthetic Biology; Professor David Karig, Johns Hopkins University

  (Topic: *The Skin-Microbe Interactome*; Dr. Virginia Pasour, Mathematical Sciences and Dr. Wallace Buchholz, Life Sciences)

- Precision Chemical Dynamics and Quantum Control of Ultracold Molecular Ion Reactions; Professor Eric Hudson, University of California - Los Angeles
  (Topic: *Ultracold Molecular Ion Reactions*; Dr. Paul Baker, Physics, and Dr. James Parker, Chemical Sciences)
- Post-Born-Oppenheimer Dynamics Using Isolated Attosecond Pulses; Professor Stephen Leone, University of California - Berkeley
  (Topic: *Attosecond Molecular Dynamics*; Dr. James Parker, Chemical Sciences and Dr. Richard Hammond, Physics)
- Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials; Professor Mitchell Luskin, University of Minnesota - Minneapolis
  (Topic: *Strongly Linked Multiscale Models for Predicting Novel Functional Materials*; Dr. Joseph Myers, Mathematical Sciences, and Dr. Chakrapani Varanasi, Materials Science)
- New Theoretical and Experimental Methods for Predicting Fundamental Mechanisms of Complex Chemical Processes; Professor Donald Thompson, University of Missouri - Columbia
  (Topic: *Nonlinear Dynamics of Energy Hypersurfaces Governing Reaction Networks*; Drs. Ralph Anthenien and Samuel Stanton, Mechanical Sciences)
- Bio-inspired Design of Adaptive Catalysis Cascades; Professor Shelley Minteer, University of Utah
  (Topic: *Multistep Catalysis*; Dr. Robert Mantz, Chemical Sciences, and Dr. David Stepp, Materials Science)
- Mechanisms of Prokaryotic Evolution; Professor Michael Lynch, Indiana University - Bloomington
  (Topic: *Innovation in Social Organisms*; Dr. Micheline Strand, Life Sciences, and Dr. John Lavery, Mathematical Sciences)

The following topics were published in FY14 and constitute the ARO portion of the FY15 MURI BAA. The topic titles, topic author(s), and corresponding ARO Division(s) are listed below.

- *Emulating the Principles of Impulsive Biological Force Generation*; Dr. Samuel Stanton, Mechanical Sciences, and Dr. Robert Kokoska, Life Sciences
- *Exploiting Nitrogen Vacancy Diamonds for Manipulation of Biological Transduction*; Dr. Frederick Gregory, Life Sciences, and Dr. Paul Baker, Physics
- *Noncommutativity in Interdependent Multimodal Data Analysis*; Dr. Liyi Dai, Computing Sciences, and Dr. T.R. Govindan, Physics
- *Multi-scale Response for Adaptive Chemical and Material Systems*; Dr. Jennifer Becker, Chemical Sciences, and Dr. John Prater, Materials Science
- *New Regimes in Quantum Optics*; Dr. T.R. Govindan, Physics, and Dr. Joe Qiu, Electronics
- *Fractional Order Methods for Sharp Interface Flows*; Dr. Joe Myers, Mathematical Sciences, and Dr. Bryan Glaz, ARL-VTD
- *2-Dimensional Organic Polymers*; Dr. Pani Varanasi, Materials Science, and Dr. Dawanne Poree, Chemical Sciences
- *Network Science of Teams*; Dr. Kate Coronges, Network 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 outstanding 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 (S&T) that is relevant to the mission of the sponsoring organization or agency, and (ii) community service demonstrated through scientific leadership, education, and community outreach.

The PECASE winners for each calendar year are typically announced by the White House at the end of the fiscal year. However, the 2014 PECASE recipients had not yet been announced at the time this issue of ARO in Review was completed.

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 university capabilities to perform cutting-edge defense research. DURIP meets a critical need by enabling university researchers to purchase scientific equipment costing $50K or more to conduct DoD-relevant research. In FY14, the Army awarded 69 grants at $12,012,529 total, with an average award of $174K.

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 components and agencies. One DoD Service or 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 the two UARCs listed below.

- The Institute for Soldier Nanotechnologies (ISN), located at the Massachusetts Institute of Technology (MIT). The ISN is discussed further in CHAPTER 3: CHEMICAL SCIENCES DIVISION.
- The Institute for Collaborative Biotechnologies (ICB), located at the University of California - Santa Barbara, with academic partners at MIT and the California Institute of Technology. The ICB is discussed further in CHAPTER 6: LIFE SCIENCES DIVISION.

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 titles of ARO-managed Minerva projects that began in FY14 are listed below, followed by the name of the lead PI, the performing organization, and the award duration.

- *Taking Development (Im)balance Seriously: Using New Approaches to Measure & Model State Fragility*, PI: Professor Jonathan Moyer, Denver University, FY14-FY17
- *Understanding the Origin, Characteristics, & Implications of Mass Political Movements*, PI: Professor Stephen Kosack, University of Washington, FY14-FY17
- *Program on Complex Emergencies & Political Stability in Asia*, PI: Professor Joshua Busby, University of Texas - Austin, FY14-FY17
- *Household Formation Systems, Marriage Markets & Society Stability/Resilience*, PI: Professor Valerie Hudson, Texas A&M University, FY14-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 solicitation contains topics seeking specific solutions to stated government needs. Phase I proposals must respond to a specific topic in the solicitation, 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 solicitations. Typically 50% of Phase II proposals are selected for award. SBIR Phase II awards may also be selected to receive additional funds as a Phase II Enhancement or via the Commercialization Readiness Program (CRP).

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 FY14 SBIR and STTR Topics

The following SBIR and Chemical and Biological Defense SBIR (CBD-SBIR) topics were published in FY14 SBIR solicitations. The lead topic author and corresponding Division are listed following each topic title.

- *Reproducible High Yield Production of Structural Proteins for Biologically-derived Fibers As an Alternative to Nylon;* Dr. Stephanie McElhinny, Life Sciences

The following STTR topics were published in FY14 STTR solicitations. The lead topic author 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 Applications*; Dr. Chakrapani Varanasi, Materials Science

- *Technology to Regulate Circadian Rhythm for Health and Performance*; Dr. Virginia Pasour, Mathematical Sciences
- *Cryogenic Low-Noise Amplifiers for Quantum Computing and Mixed-Signal Applications*; Dr. TR Govindan, Physics
- *Freeze Casting of Tubular Sulfur Tolerant Materials for Solid Oxide Fuel Cells*; Dr. Robert Mantz, Chemical Sciences
- *Bio-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. Jim Parker, Chemical Sciences

D. ARO FY14 SBIR and STTR Phase II Awarded Topics

The following SBIR, CBD-SBIR, and OSD-SBIR topics were selected for a Phase II award in FY14. The lead topic author and corresponding Division are listed following each topic title.

- *Responsive Sequestration Coatings*; Dr. Jennifer Becker, Chemical Sciences
- *Formulation Development to Enhance Bioavailability and Pharmacokinetic Profile of Protein-based Drugs*; Dr. Jennifer Becker, Chemical Sciences
- *Advanced Purification Technology for the Manufacture of Vaccines, Biologic Drugs, and Enzymes*; Dr. Jennifer Becker, Chemical Sciences
- *Ultra-Sensitive, Room-Temperature, Mechanical-Optical-Cavity Detectors for Long-Wavelength Applications*; Dr. William Clark, Electronics
- *Rapid Analysis of Suspicious Powders*; Dr. Stephanie McElhinny, Life Sciences
- *Global Spatiotemporal Disease Surveillance System*; Dr. Stephanie McElhinny, Life Sciences
- *Fusing Uncertain and Heterogeneous Information*; Dr. Purush Iyer, Network Sciences
- *Wide Field-of-View Imaging System with Active Mitigation of Turbulence Effects for Tactical Applications*; Dr. Liyi Dai, Computing Sciences

The following STTR and OSD STTR topics were selected for a Phase II award in FY14. The lead topic author and corresponding Division are listed following each topic title.

- *Sensitive and Shape-Specific Molecular Identification*; Dr. Jim Parker, Chemical Sciences
- *Compressive Sampling Video Sensor for Change Detection*; Dr. Liyi Dai, Computing Sciences
- *Wide Temperature Range, High-Speed Optical Interconnect Technology*; Dr. Michael Gerhold, Electronics
- *Inferring Social and Psychological Meaning in Social Media*; Dr. Joseph Myers, Mathematical Sciences
- *Nanostructured Electrode Materials for Enhanced Biological Charge Transfer*; Dr. Stephanie McElhinny, Life Sciences
- *Mesh Generation and Control for Moving Boundary Problems*; Dr. Joseph Myers, Mathematical Sciences
- *Nondestructive Concrete Characterization System*; Dr. Jennifer Becker, Chemical Sciences
- *High Throughput Forensic Palynology*; Dr. Micheline Strand, Life Sciences
- *High Quality AlGaN Epitaxial Films with Reduced Surface Dislocation Density*; Dr. Chakrapani Varanasi, Materials Science
- *Atomic Layer Deposition of Lead Zirconate Titanate Thin Films for PiezoMEMS Applications*; Dr. Chakrapani Varanasi, Materials Science
- *Liquid Crystal-based Sensors for Detection of Airborne Toxic Chemicals for Integration with Unmanned Robotic Systems*; Dr. Jennifer Becker, Chemical Sciences
- *Solar-blind (Be,Mg)ZnO Photodetectors (260-285 nm wavelengths)*; Dr. William Clark, Electronics
- *Non-Deteriorating Numerical Simulation of 3D Unsteady Wave Phenomena over Long Times*; Dr. Joseph Myers, Mathematical Sciences

- *Near Real-Time Quantification of Stochastic Model Parameters*; Dr. Joseph Myers, Mathematical Sciences
- *Effective Cyber Situation Awareness Assessment and Training*; Dr. Cliff Wang, Computing Sciences

E. ARO FY14 SBIR Phase III Awarded Topics

The following SBIR topics were awarded a Phase III contract in FY13 and FY14. The lead topic author and corresponding Division are listed following each topic title. Phase III revenues can be obtained from Government or private customers, but cannot be SBIR funds.

- *Rapid, Quantitative Biological Indicator System with Bacillus thuringiensis Al Hakam Spores(1001-810)*; Dr. Jennifer Becker, Chemical Sciences
- *Multisensory Navigation and Communications System*; Dr. Fredrick Gregory, Life Sciences
- *Research and Development Supporting New EW Capabilities*; Dr. James Harvey, Electronics
- *Equipment Sets for Mitigating Advanced Threats*; Dr. Stephen Lee, Chemical Sciences

F. 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 specific solicitation periods throughout each fiscal year. Proposals are evaluated against published evaluation criteria and selected for contract award. Contract awards in the SBIR and STTR programs 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.

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

Programs for HBCU/MIs are a significant part of the ARO portfolio. Awards in FY14 totaled $15.6 million. These programs are discussed in the following subsections.

A. ARO (Core) HBCU/MI Program

ARO began its HBCU/MI program in 1980 with $0.5 million designed to encourage greater participation of HBCUs and MIs 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/MI research proposals submitted through the ARO Core Program BAA. There were 31 agreements with HBCU/MI institutions receiving over $2.3 million in funding through the ARO Core Program during FY14, including the 14 new starts. These figures represent total funding for HBCU/MIs through the core program, both awards relying on matching funds and those not utilizing matching funds.

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

- *Bio-inspired Structured Graphical Models for Inference and Information Fusion*, Professor Mohamed Chouikha, Howard University; Dr. Joseph Myers, Mathematical Sciences
- *Warfighter Neuroendocrinology: Modeling stress response, PTSD, and TBI*, Professor Maria-Rita D'Orsogna, California State University - Northridge; Dr. Virginia Pasour, Mathematical Sciences
- *Scalable Algoritlnns Based on Abstraction for Adversarial Reasoning under Uncertainty*, Professor Christopher Kiekintveld, University of Texas - El Paso; Dr. Purush Iyer, Network Sciences

- *Microwave and Terahertz Applications of Two-Dimensional Electron Systems*, Professor Ramesh G. Mani, Georgia State University; Dr. Joe Qiu, Electronics Division
- *TL/OSL Dating: Lattice Structure, Dating Accuracy, and Temporal Minima*, Professor David Sammeth, New Mexico Highlands University; Dr. David Stepp, Materials Science
- *Optimized Energy Management of Heat Transport in Smallest Engines: A Quantum Thermodynamic Approach*, Professor Ilki Kim, NC A&T State University; Dr. Robert Mantz, Chemical Sciences
- *Investigation of the Decomposition of Energetics Materials*, Professor Ralf Kaiser, University of Hawaii; Dr. James Parker, Chemical Sciences
- *Control of Light-Matter Interactions with Metamaterials*, Professor Mikhail Noginov, Norfolk State University; Dr. Richard Hammond, Physics Division
- *Creating Magnetic Plasmons at Visible Frequencies: Towards Isotropic Negative Index Metamaterials*, Professor Ming Tang, University of California - Riverside; Dr. John Prater, Material Sciences
- *Sensitive Indicators and Risk Factors of Blast-Induced Neurodegeneration in Hippocampus,* Professor Ben Bahr, University of North Carolina at Pembroke; Dr. Frederick Gregory, Life Sciences
- *Experimental Investigation of the Micromechanics of Rock Damage During Dynamic Loading Events (ARO Research Are 2.1: Terrestrial Sciences)*, Professor William Griffith, University of Texas at Arlington; Dr. David Stepp, Materials Science
- *Rapid Characterization of Spider Silk Genes via Exon Capture (ARO topic area 8.2 Molecular Genetics),* Professor Cheryl Hayashi, University of California - Riverside; Dr. Micheline Strand, Life Sciences
- *Data-driven Dynamic Modeling of Activity-dependent Regulation in the STG Pyloric Circuit*, Professor Robert Clewley, Georgia State University; Dr. Virginia Pasour, Mathematical Sciences
- *Chemical Transformations via Photon-induced Metal-to-molecule E^- Transfer at Metal Nanocrystals,* Professor Phillip Christopher, University of California - Riverside; Dr. Robert Mantz, Chemical Sciences

The HBCU/MI 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 twelve HBCU/MIs were funded under HSAP/URAP in FY14, totaling approximately $77K, (50/50 mix of program manager 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 FY14, $1.3 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

- *Nano to Continuum 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/MI

ARO has administered programs on behalf of ASD(R&E) since 1992. REP aims to enhance research capabilities of HBCUs and MIs and to strengthen their education programs in science, technology, engineering, and mathematics (STEM) disciplines that are relevant to the defense mission. The FY14 BAA solicited proposals from single investigators for the acquisition of equipment and instrumentation to augment existing research and education capabilities and/or to develop new capabilities. Proposals were limited to two per eligible institution.

Under this program, qualifying institutions were able to submit proposals to compete for research equipment/instrumentation grants. In 3Q FY14, BAA W911NF-14-R-0009 was issued for the FY14 DoD REP for HBCU/MI. Ninety (90) proposals were determined to be eligible under the solicitation. In FY14, 33 grants totaling $10.7 million were made to 13 HBCUs, 18 MIs, and 2 TCUs under the DoD REP solicitation."

D. DoD Instrumentation Program for Tribal Colleges and Universities (TCUs)

There was no instrumentation program for TCUs in FY14.

E. Other HBCU/MI Activities

ARO was selected to administer the Congressionally-directed program "STEM Research and Veteran Technology Workforce Development Initiatives" for an HBCU institution located in South Carolina. Funding for this FY10 statutory add totaled $2.0 million and was awarded to Benedict College in Columbia, SC in 3Q FY11. The program ended in FY14. In addition, the John H. Hopps Scholars Program at Morehouse College (funded in FY08) continued to serve eight scholars during FY14. The Hopps Program ends in August 2016.

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

The NDSEG Fellowship Program is an OSD-funded program administered by 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 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, and up to $1K/year in medical insurance.

With approximately $5 million available to the Army in FY14, ARO selected 64 NDSEG Fellows from thirteen categories relevant to Army fundamental research priorities. These awardees began their fellowships in the fall of 2013. 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 FY14 NDSEG program is shown in TABLE 2.

TABLE 2

FY14 NDSEG fellows by discipline. The table displays the number of NDSEG Fellows chosen in FY14, according to topic categories relevant to the designated Army research priorities.

Scientific Discipline	NDSEG Fellows Selected in FY14
Aeronautical and Astronautical Engineering	4
Biosciences	12
Chemical Engineering	4
Chemistry	5
Civil Engineering	3
Cognitive, Neural, and Behavioral Sciences	5
Computer and Computational Sciences	4
Electrical Engineering	4
Geosciences	3
Materials Science and Engineering	6
Mathematics	3
Mechanical Engineering	6
Physics	5
TOTAL	**64**

XI. YOUTH SCIENCE ACTIVITIES

With the departure of ARO's youth science program manager early in FY14, several of the Army Educational Outreach Program (AEOP) programs that were managed by ARO in previous years were transferred and managed by the STEM Outreach Office at RDECOM Headquarters for the remainder of FY14. All the programs 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 administered High School and Undergraduate Research Apprenticeship Programs and managed the funding of and modifications to the Youth Science Cooperative Outreach Agreement (YS-COA).

During the summer of FY14, 69 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). 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 FY14, URAP awards provided 59 students with research experiences at 27 different universities within 17 different states. Six of the universities were HBCU/MIs and ARO invested approximately $210K in the FY14 HSAP 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 FY14, HSAP awards provided 10 students with research experiences at 7 different universities within 7 different states. Three of the universities were HBCU/MIs. ARO invested approximately $38.5K in the FY14 HSAP effort, a mix of ARO core funding and AEOP matching funds.

C. Youth Science Cooperative Outreach Agreement (YS-COA)

The YSCOA completed its fourth year of outreach efforts in FY14. It was awarded on 30 September 2010 to provide support and stimulation of STEM education and outreach in conjunction with DoD and the Army. YS-COA brings together government and a consortium of organizations working collaboratively to further STEM education and outreach efforts nationwide and consists of twelve major components, including the Junior Science and Humanities Symposium (JSHS), the Research and Engineering Apprenticeship Program (REAP), UNITE, Junior Solar Sprint (JSS), the Science and Engineering Apprentice Program (SEAP), College Qualified Leaders (CQL), Gains in the Education of Mathematical Sciences and Science (GEMS), ECybermission Internship Program (ECIP), and a strategic overarching marketing and metrics collection and evaluation effort. As mentioned above, ARO's Co-Cooperative Agreement Manager (CAM) role migrated to RDECOM HQ in early FY14 as did the programs for which ARO had the lead role (except HSAP and URAP).

Virginia Polytechnic Institute and State University has led the consortium of non-profits and academic institutions to execute a collaborative STEM education and outreach program focusing on the Army Educational Outreach Program (AEOP) core objectives:

- STEM Literate Citizenry: Broaden, deepen, and diversify the pool of STEM talent in support of our Defense Industry Base (DIB)
- STEM "Savvy" Educators: Support and empower educators with unique Army Research and Technology Resources
- Develop and implement a cohesive, coordinated, and sustainable STEM education outreach infrastructure across the Army

The major accomplishments in FY14 included year-end program reviews with Individual Program Agents (IPAs), Cooperative Agreement Consortium Meeting and Army Cooperative Agreement and subject matter experts, as well as the release of the AEOP Abstract Book, and AEOP Marketing Products.

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 FY14, 65 new SSP tasks were awarded in addition to 165 modifications of the scope and/or funding of ongoing tasks on two SSP contracts. A summary of the agencies served under this program and the corresponding number of FY14 new SSP tasks is provided in TABLE 3.

TABLE 3
FY14 SSP tasks and sponsoring agencies.

Sponsoring Organization	SSP Tasks
Army Research, Development and Engineering Command (RDECOM)	
Army Research Laboratory (ARL)	11
Edgewood Chemical, Biological Center (ECBC)	2
Army Materiel Systems Analysis Activity (AMSAA)	1
Research, Development, and Engineering Centers (RDECs)	
Army Missile RDEC (AMRDEC)	5
Natick Soldier RDEC (NSRDEC)	4
Communications-Electronics RDEC (CERDEC)	4
Tank Automotive RDEC (TARDEC)	2
TOTAL: RDECOM	**29**
Other U.S. Army	
US Military Academy (USMA)	4
Headquarters Department of Army (HQ DA)	6
Program Executive Office Combat Support & Combat Service Support	1
US Army Corps of Engineers (USACE)	8
US Army Training & Doctrine Command (TRADOC)	2
Program Executive Office Ground Combat Systems (PEO-GCS)	1
TOTAL: Other U.S. Army	**22**
Other DoD	
US Air Force	7
US Navy	5
DoD (Other)	2
TOTAL: Other DoD	**14**
TOTAL FY14 SSP Tasks	**65**

XIII. SUMMARY OF PROGRAM FUNDING AND ACTIONS

A. FY14 Research Proposal Actions

The FY14 extramural basic research proposal actions for each ARO Division are summarized in TABLE 4, below.

TABLE 4

FY14 ARO Research Proposal Actions. The status of research proposals received within FY14 (*i.e.*, 1 Oct 2013 through 30 Sep 2014) is listed for each scientific division, based on proposal actions reported through 4 Jun 2015. The table reports actions for extramural proposals in the 6.1 basic research categories: SI, STIR, YIP, HBCU/MI Core, MRI, MURI, PECASE, and DURIP.

	Received	Accepted	Declined	Pending	Withdrawn
Chemical Sciences	90	39	28	23	0
Computing Sciences	46	35	3	8	0
Electronics	85	43	30	12	0
Life Sciences	128	58	43	26	1
Materials Science	133	54	43	35	1
Mathematical Sciences	67	43	7	17	0
Mechanical Sciences	89	30	39	16	4
Network Sciences	68	39	12	15	2
Physics	63	33	22	8	0
TOTAL	**769**	**374**	**227**	**161**	**8**

B. Summary of ARO Core Program Budget

The ARO FY14 Core (BH57) Research Program budget is shown in TABLE 5, below.

TABLE 5

ARO Core (BH57) Program funding. The ARO Core Program FY14 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 31 Jan 2015 (for special programs).

ARO Core (BH57) Program Type	Division or Program Title	FY14 Allotment
Scientific Disciplines	Chemical Sciences	$7,072,258
	Computing Sciences	$5,182,720
	Electronics	$6,282,200
	Environmental Sciences (Legacy)[1]	$2,506,900
	Life Sciences	$7,324,500
	Materials Science	$6,958,000
	Mathematical Sciences	$5,646,850
	Mechanical Sciences	$6,909,500
	Network Sciences	$5,829,080
	Physics	$6,791,750
	SUBTOTAL: Core Program Funding by Scientific Discipline	**$60,503,758**
Special Programs	Senior Scientist Research Programs	$882,873
	ARL Fellows' Stipends	$75,000
	National Research Council (NRC) Associates Program	$235,455
	HBCU/MI Program[2,3]	$645,000
	HSAP/URAP	$495,000
	In-House Operations	$14,827,257
	SUBTOTAL: Core Program Funding to Special Programs	**$17,160,585**
TOTAL	**ARO Core (BH57) Program**	**$77,664,343**

[1] The Environmental Sciences Division began a reorganization process in FY14; this amount represents funding for projects that began in earlier years.

[2] HBCU/MI Core Program funds are allocated at the Directorate level, and are matched with Division funds, resulting in total FY14 HBCU/MI Core Program funding of $1.3M.

[3] This table does not include the additional funds provided from OSD for the HBCU/MI Program (see TABLE 8).

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

The FY14 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

FY14 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: 31 Jan 2015 Status of Funds Report.

Other Army-funded Program	FY14 Allotment
Multidisciplinary University Research Initiative	$54,624,381
Presidential Early Career Award for Scientists and Engineers	$4,393,988
Defense University Research Instrumentation Program	$12,012,529
University Research Initiative Support	$2,426,000
MINERVA Program (Project V72)[1]	$3,225,177
Army Center of Excellence (Project H59)	$976,298
HBCU/MI – PIRT Centers (Project H04)	$3,612,952
Institute for Collaborative Biotechnologies (ICB; Project H05)	$12,037,376
Institute for Soldier Nanotechnologies (ISN; Project J12)	$10,927,427
Institute for Creative Technologies (ICT; Project J08)	$7,829,950
Board of Army Science and Technology (BAST; Project C18)	$614,872
Small Business Innovation Research (SBIR; Project M40)[1,2]	$6,938,048
Small Business Technology Transfer (STTR; Project 861)[1,3]	$13,839,896
SBIR/STTR Services / Contract Support (Project 720)	$854,392
Research In Ballistics (Project H43)	$1,247,882
Communications and Electronics RDEC (CERDEC)	$6,321,298
Other Army (*e.g.*, Rapid Equipping Force)	$63,527,831
TOTAL: Other Army-funded Programs	**$205,410,297**

[1] Does not include additional funds provided by OSD (see TABLE 8).
[2] Includes $5,158,444 of FY13 funds received in or reallocated for FY14
[3] Includes $4,339,517 of FY13 funds received in or reallocated for FY14

TABLE 7

FY14 allotment for externally-funded programs. FY14 funds received from sources other than Army or OSD are indicated below; data source: 31 Jan 2015 Status of Funds Report. 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.

External Program	FY14 Allotment
Scientific Services Program (SSP)[1]	$17,912,608
Defense Advanced Research Projects Agency (DARPA)[2]	$161,281,293
Other Agencies (*e.g.*, JIEDDO and JPMNBC)[3]	$56,584,991
TOTAL: External Programs	**$235,778,892**

[1] Includes $3,844,611 of FY13 funds received in or reallocated for FY14
[2] Includes $21,613,033 of FY13 funds received in or reallocated for FY14
[3] Includes $6,685,120 of FY13 funds received in or reallocated for FY14

TABLE 8

OSD direct-funded programs. These funds were allocated directly from OSD to the indicated program; data source: 31 Jan 2015 Status of Funds Report.

OSD Direct-funded Programs	FY13 Allotment
SBIR/STTR (Project 8Z5)[1,2]	$2,023,668
HBCU/MI and Research and Educational Program (REP)[3]	$14,990,000
Chemical and Biological Defense Programs (Project BP0)[4]	$8,387,997
MINERVA	$5,060,000
TOTAL: OSD Direct Funding	**$26,755,254**

[1] Does not include additional Army funds provided for SBIR/STTR (see TABLE 6).
[2] FY13 funds received in or reallocated for FY14
[3] This amount does not include the additional Army Core Program funds provided for the HBCU/MI Program (see TABLE 5).
[4] Includes $5,324,141 of FY13 funds received in or reallocated for FY14

D. Grand Total FY14 Allotment for ARO Managed or Co-managed Programs

TABLE 9

Summary of FY14 allotment for all ARO managed or co-managed programs. This table lists the subtotals from TABLES 6-9 and the grand total FY14 allotment for all ARO managed or co-managed programs, including any FY13 funds received in or allocated for FY14.

Program Category	FY14 Allotment
Core (BH57) Programs	$77,664,343
Other Army-funded Programs	$205,410,297
External Program Funds	$235,778,892
OSD Direct-funded Programs	$26,755,254
GRAND TOTAL: (all sources)	**$545,608,786**

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 2014* is to provide information on the programs and basic research supported by ARO in FY14, and ARO's long-term vision for transitioning 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 basic-to-applied research transitions facilitated by this Division in FY14.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Chemical Sciences Division supports research to advance the Army and nation's knowledge and understanding of the fundamental properties, principles, and processes governing molecules and their interactions in materials or chemical systems. 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. In addition to advancing world-wide knowledge and understanding of chemical processes, research in 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. Research in chemical sciences 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. Research in the Chemical Sciences Division is also coordinated with research in the Atmospheric Sciences Program (of the former Environmental Sciences Division; refer to CHAPTER 1, Section V), in which new methods and reactions are being explored for detecting, identifying, and neutralizing toxic materials. These interactions promote a synergy among ARO Divisions, providing a more effective mechanism for meeting the long-term needs of the Army.

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 FY14, the Division managed research within these four 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. Within these thrusts, high-risk, high-payoff research is identified and supported to pursue the Program's long-term goal. 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, fuel cell membranes to harness renewable energy, and damage-sensing and self-healing materials for vehicles, aircraft, and other DoD materiel. 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 primary 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 (temperatures and pressures), and to develop theories that are 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 research Thrusts: (i) Molecular Dynamics and (ii) Quantitative Theoretical Methods. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high-payoff research efforts. The Molecular Dynamics Thrust broadly supports research on the study of energy transfer mechanisms in molecular systems (reactive and non-reactive). 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 for the Army and general public. These applications include more efficient and clean combustion technology, the development of new tools to study condensed phases of matter, 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 basic 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 and Electrocatalysis, and (ii) Transport of Electroactive Species. These Thrust areas guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Redox Chemistry and Electrocatalysis Thrust supports research efforts to discover new 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 also 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 FY14 were $63.4 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY14 ARO Core (BH57) program funding allotment for this Division was $7.1 million. 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 $12.9 million to projects managed by the Division. The Division also managed $3.0 million of Defense Threat Reduction Agency (DTRA) programs, $15.8 million of Defense Advanced Research Projects Agency (DARPA) programs, and $1.0 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $2.9 million for contracts. The Institute for Soldier Nanotechnologies received $18.9 million. Finally, $1.8 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.2 million of 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 FY14 (*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 FY14 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 FY14, the Division awarded 19 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to characterize chemical processes at surfaces, to understand previously-unknown chemical reaction mechanisms, and to create new types of functionalized polymers. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Nicholas Abbott, University of Wisconsin – Madison; *Role of Interfacial Ionic Phenomena in Controlling the Ordering of Liquid Crystals*
- Professor Joel Bowman, Emory University; *Theoretical Studies of "Roaming" Chemical Reactions*
- Professor Adam Braunschweig, University of Miami - Coral Gables; *Synergistic Approaches to Functional Self-Assembling Aggregates*
- Professor Laurie Butler, University of Chicago; *Radical Reactions in the Decomposition of Geminal Di-Nitro Energetic Materials*
- Professor Peng Chen, Cornell University; *Catalytic Reactivity at Nanoscale Metal-Metal Interfaces*
- Professor Peng Chen, Cornell University; *Tracking Living Polymerization at the Single-Molecule Level*
- Professor Wilson Chiu, University of Connecticut - Storrs; *Carbonate and Hydroxide Ion Transport in Alkaline Anion Exchange Materials*
- Professor Stephen Cronin, University of Southern California; *Surface Intermediates and Reaction Mechanisms in Photoelectrochemistry on Plasmon Resonant Metal/Semiconductor Nanostructures*
- Professor Yossef Elabd, Texas Engineering Experiment Station; *Highly Conductive Anion Exchange Block Copolymers*
- Professor Todd Emrick, University of Massachusetts - Amherst; *Responsive Polymer Assembly at the Mesoscale*
- Professor Haifeng Gao, University of Notre Dame; *Regulating Inter-Polymer Chain Reaction in Nanospace: an Efficient Method to Produce Hyperbranched Polymer with Uniform Structure*
- Professor Nathan Gianneschi, University of California - San Diego; *Propagating Molecular Recognition Events through Highly Integrated Sense-Response Chemical Systems*

- Professor Weiguo Hu, University of Massachusetts - Amherst; *High-Resolution Measurements of Polymer Molecular Dynamics by Novel Solid-State NMR Methods*
- Professor Nicholas Leventis, Missouri University of Science and Technology; *Fractal Assembly of Polymeric Nanoparticles into Fibers versus Globules: an Experimental and Computational Study*
- Professor Rudolph Marcus, California Institute of Technology; *Novel Surface Phenomena*
- Professor John Morris, Virginia Polytechnic Institute & State University; *Photocatalysis at TiO_2-Supported Au Nanoparticles: Studies of Thermal, UV, and Visible Energy-Driven Chemistry*
- Professor William Phillip, University of Notre Dame; *Understanding the Novel Stimuli Responsive Transport Properties of Multifunctional, Nanostructured Block Polymer Membranes*
- Professor Scott Phillips, Pennsylvania State University; *Polymers that Depolymerize From Head-to-Tail in the Solid State*
- Professor Greg Swain, Michigan State University; *Electrochemistry of Nanostructured Carbon Electrodes in Room-Temperature Ionic Liquids*

2. Short Term Innovative Research (STIR) Program. In FY14, the Division awarded 11 new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to synthesize ionically-crosslinked elastomers and to measure the surface interactions of enzymes at single-molecule resolution. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Andrew Boydston, University of Washington; *Development of Thermally- and Mechanically-Triggered Self-Immolative Polymers*
- Professor Kevin Cavicchi, University of Akron; *Synthesis and Characterization of Ionically Crosslinked Elastomers*
- Professor David Go, University of Notre Dame; *Probing Electrochemical Reactions at a Plasma-Liquid Interface*
- Professor Robert Grubbs, Research Foundation of SUNY - Stony Brook University; *Degradable Polymers and Block Copolymers from Electron-deficient Carbonyl Compounds*
- Professor Joel Kaar,University of Colorado – Boulder; *Single Molecule Resolution of Surface Interactions of an Evolved Enzyme*
- Professor Michael Kilbey, University of Tennessee - Knoxville; *Synthesis of Novel Purine-based Polymers*
- Professor Ilki Kim, North Carolina A&T State University; *Optimized Energy Management of Heat Transport in Smallest Engines: A Quantum Thermodynamic Approach*
- Professor John Matson, Virginia Polytechnic Institute & State University; *Tapered Bottlebrush Polymers: A New Polymer Architecture*
- Professor Ajay Prasad, University of Delaware; *Improved Electrolyte Surface Exchange via Atomically Strained Surfaces*
- Professor Eugene Smotkin, Northeastern University; *Acid Strength Tuning of Heterogeneous Catalysts by Potential Control*
- Professor Yan Xia, Stanford University; *Chain Growth Cross Coupling Polymerizations Towards Chiral and Ladder Main Chain Polymers*

3. Young Investigator Program (YIP). In FY14, the Division awarded three new YIP projects. These grants are driving fundamental research such as studies to design and synthesize linear polymers that fold into architecturally-defined 3D nanostructures and to understand energy transfer on metal-nanoparticle surfaces. The following PIs and corresponding organizations were recipients of new-start YIP awards.

- Professor Erik Berda, University of New Hampshire; *Origami of Single Polymer Chains via Sequentially Activated Permanent and Reversible Intra-chain Interactions*
- Professor Phillip Christopher, University of California - Riverside; *Chemical Transformations via Photon Induced Metal-to-Molecule Electron Transfer at Metal Nanocrystal Surfaces*
- Professor Brian Long, University of Tennessee at Knoxville; *Redox-Switchable Coordination Catalysis: An Advanced Tool for Catalyst Control and Tailored Polyolefin Synthesis*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY14 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *13th Polymer Electrolyte Fuel Cell Symposium at the 226th International Meeting of the Electrochemical Society*; Cancun, Mexico; 5-10 October 2013
- *19th International Symposium on Molten Salts and Ionic Liquids at the 226th International Meeting of the Electrochemical Society*; Cancun, Mexico; 5-10 October 2013
- *13th Polymer Electrolyte Fuel Cell Sympoium at the 224th Eelctrochemical Society Meeing*; San Francisco CA location; 27 Oct - 1 Nov 2013
- *Symposium Z: Materials Challenges for Energy Storage Across Multiple Scales at the Materials Research Society Fall Meeting*; Boston, MA; 30 November - 5 December 2013
- *2014 Electrochemistry Gordon Research Conference: Five Decades of Impact and Sustained Growth*; Ventura, CA; 5-10 January 2014
- *Batteries Gordon Research Conference*; Ventura, CA; 8-14 March 2014
- *Electrochemical Conference on Energy and the Environment*; Shanghai, China; 13-16 March 2014
- *Advances in Olefin Polymerization Catalysis Symposium at the ACS National Meeting*; Dallas, TX; 16-20 March 2014
- *Shape Programmable Materials Symposium at the Materials Research Society Spring Meeting*; San Francisco, CA; 21-25 April 2014
- *Crystal Engineering Gordon Research Conference*; Waterville Valley, NH; 1-6 June 2014
- *Flexible SERS Substrates: Challenges and Opportunities;* St. Louis, MO; 25-26 June 2014
- *Colloidal Semiconductor Nanocrystals Gordon Research Conference*; Smithfield, RI; 20-25 July 2014
- *Electrodeposition Gordon Research Conference*; Biddeford, ME; 27 July - 1 August 2014
- *Fuel Cells Gordon Research Conference*; Smithfield, RI; 2-9 August 2014
- *Modeling And Simulations Of Electrochemical Interfaces And Materials For Energy Storage Symposium at the ACS National Meeting*; San Francisco, CA; 10-14 August 2014
- *Responsive Supramolecular, Macromolecular and Nanostructured Systems and Biopolymer-driven Organization of Nanostructures at the ACS National Meeting*; San Francisco, CA; 10-14 August 2014
- *Stimuli-Responsive Supramolecular, Macromolecular and Nanostructured Systems and Biopolymer-Driven Organization of Nanostructures Symposium at the ACS National Meeting*; San Francisco, CA; 10-14 August 2014
- *Targeting and Triggering Basic Research Workshop and Review;* Cambridge, United Kingdom, 19-20 August 2014
- *Nanotechnology to Aid Chemical and Biological Defense;* Antalya, Turkey; 23-25 September 2014

5. Special Programs. In FY14, 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 three 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. Molecular Design of Novel Fibers using Carbon Nonotubes. This MURI began in FY09 and was awarded to a team led by Professor Horacio Espinosa at Northwestern University. The focus of this MURI is to understand the molecular properties required for preparing strong fibers using polymers and double-walled carbon nanotubes (DWCNT).

The chief objectives of this research are to (i) develop a model system for predicting the molecular properties necessary for preparing new, high-strength fibers, and (ii) to prepare novel fibers composed of double-walled carbon nanotubes and polymers. The team will use multiscale computer simulations to bridge atomistic (*i.e.*, electronic structure methods and reactive force fields), coarse-grain, and continuum scales to explore and understand DWCNT-polymer interactions, crosslinking effects (bond-breaking mechanisms), and the impact of architecture on fiber strength, elasticity, and toughness. The investigators will use the results to predict fiber precursor properties necessary for optimum strength. The team will use predictive models to develop chemical vapor deposition techniques for producing highly-aligned DWCNT mats with optimized density and surface chemistry. The mats will serve as precursors for fiber formation. These materials will be characterized using *in situ* and *ex situ* microscopy (*i.e.*, assayed during and after reaction completion). The fundamental scientific knowledge uncovered through this research may lead to new approaches for designing and preparing high-strength, flexible fibers that are directly relevant to lighter-weight and flexible personnel armor.

2. 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.

3. 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.

4. 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.

5. 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.

6. 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.

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

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.

7. 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 Chemical 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).

8. 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.

9. 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.

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 FY14, the Division managed three new-start Phase II 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 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 FY14, the Division managed seven new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of four Phase I contracts and 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 FY14, the Division managed one new ARO (Core) HBCU/MI project and seven 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 PECASE winners for each calendar year are typically announced by the White House at the end of the fiscal year. However, the 2014 PECASE recipients had not yet been announced at the time this issue of ARO in Review was completed. 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 FY14, the Division managed 12 new DURIP projects, totaling $1.9 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

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

The ISN, 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 500 nanometers. The research performed at the ISN falls into five Strategic Research Areas (SRAs): (i) Lightweight, Multifunctional Nanostructured Materials (ii) Soldier Medicine, (iii) Blast and Ballistic Threats, (iv) Hazardous Substances Sensing, and (v) Nanosystems Integration. Each SRA is further divided into research themes. Detailed descriptions of each SRA and its corresponding themes are available at the ISN program website (http://mit.edu/isn/research/index.html).

In FY14, the ISN supported 50 faculty, 101 graduate students, and 59 postdoctoral fellows across 17 departments at MIT. The ISN program is unique in that it currently has 13 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 annually review the ISN research portfolio, assessing the goals of the various projects and research results. The ISN 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 $18.8 million of program funds was allocated to the ISN in FY14, which was the second year of a contract that was renewed in FY12 for a five-year period. Of these FY14 funds, $14.5 million was allocated for 6.1-basic research and $4.3 million was allocated for three applied-research projects, including two new projects.

I. DARPA Biofuels Alternative Feedstocks

The Biofuels Alternative Feedstocks program is developing affordable alternatives to petroleum-derived JP-8 without using algae and cellulosic biomass. The Division’s Electrochemistry Program aids in the management of this this DARPA program. DARPA seeks to conduct a one-year demonstration of state of the art algae oil production to determine current economic maturity.

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. Characterization of Nanoporous Silicon as a Medium for Size-Selective Filtration, Preconcentration, and Detection of Biomolecules

Professor Sharon Weiss, Vanderbilt University, PECASE

The goal of this research is to investigate the fundamental properties of the bio-nano interface of nanoporous materials using porous silicon as a model material. Porous silicon waveguides were selected as model materials because of their many valuable properties. For example, their high surface areas allow for increased functionalization; tuning the pore size can lead to the ability to pre-concentrate and filter molecules by size; and porous silicon waveguides utilize strong field confinement in the region where molecules are captured which increases the light-matter interaction and thus ultimately sensitivity. Previous work demonstrated the ability to functionalize the porous silicon waveguides with thiol modified probe DNA and monitor DNA hybridization by direct measurement of the resonance angle shift in the waveguide.

In FY14, the research team expanded this concept to include Peptide Nucleic Acids (PNA). PNA are synthetic nucleic acid analogs with charge-neutral amide linkages in the backbone, offering greater binding affinity for complimentary oligos and increased stability to degradation when compared to more traditional DNA and RNA. Porous silicon waveguides were functionalized with PNA by three methods, in-situ synthesis, direct nucleic acid conjugation, and physical adsorption (see FIGURE 1). Optical thickness measurements were used to determine the amount of PNA loaded within the porous silicon waveguide. PNA loading from in-situ synthesis was 8-fold greater than the amount achieved by direct conjugation and similar to the amount achieved by physical adsorption. Even though high loading was achieved through physical adsorption, for applications in biosensing, PNA probes must be stably bound to the porous silicon surface.

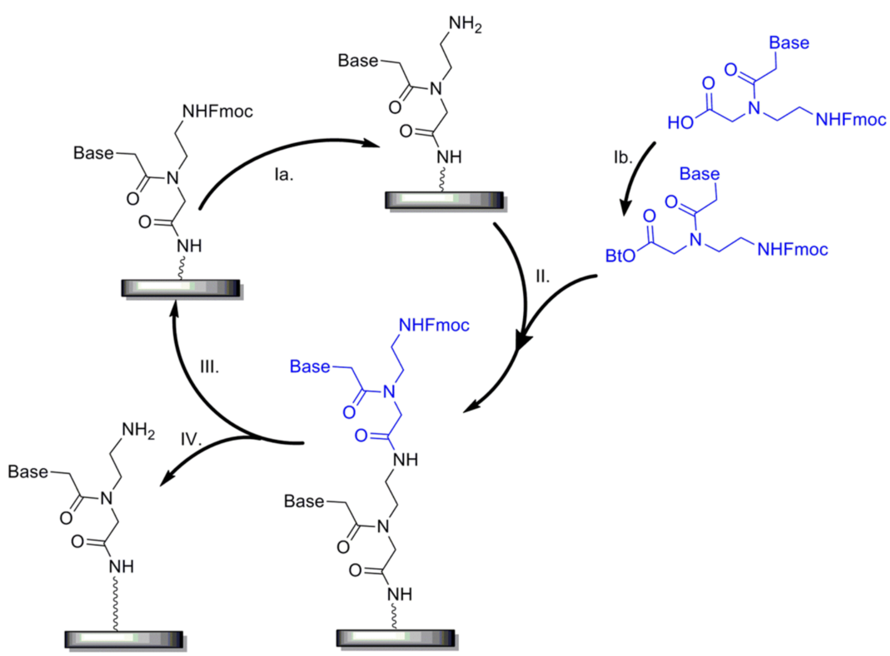

FIGURE 1

In-situ synthesis of PNA from a porous silicon solid support.

The research team demonstrated biosensor selectivity by incubating the functionalized porous silicon with buffer, 100% complimentary DNA target, or a 100% mismatch DNA sequence. The optical thickness of physical adsorption samples was found to decrease, indicating instability of the sensor surface (see FIGURE 2). However the optical thickness of the in-situ synthesized samples remained stable unless target DNA was present, in which case the thickness increased, indicating complementary probe sequence binding. Complimentary PNA oligo binding was also confirmed by observation of the waveguide resonance shift (see FIGURE 3). Future work will continue to explore the use of this functionalization platform for biosensing and drug delivery.

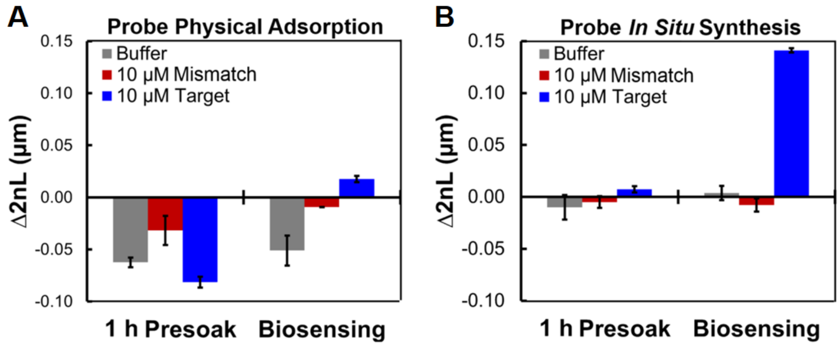

FIGURE 2

Hybridization assay following either (A) physical adsorption, or (B) in situ synthesis of a 16-mer PNA on a single-layer porous silicon biosensor.

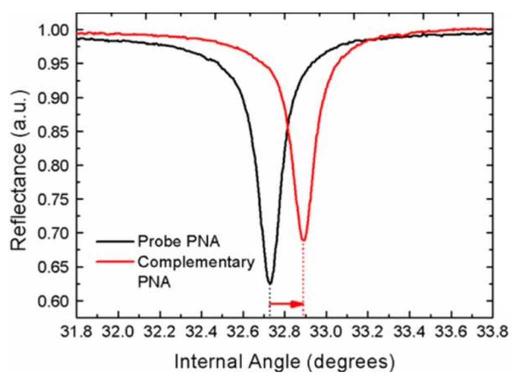

FIGURE 3

Resonance shift for a PNA probe functionalize porous silicon waveguide after incubation with 100% complementary PNA oligo target.

B. Donor-Acceptor Superstructures with Emergent Optoelectronic Properties: Synergistic Approaches to Functional Self-Assembling Aggregates

Professor Adam Braunschweig, University of Miami - Coral Gables, Single Investigator Award

The objective of this effort is to design, synthesize, and characterize self-assembled systems based on electron donor and acceptor materials, and then study responses to external stimuli. The team has developed a novel molecular system composed of diketopyrrolo pyrrole (DPP) electron donors and perylene-derived bisdiimide (PDI) electron acceptors that assemble into donor-acceptor helical superstructures as a result of multiple noncovalent interactions operating in unison. Orthogonal noncovalent interactions were programmed into these compounds to drive the supramolecular assembly of DPP and PDI (see FIGURE 4). Variable-temperature circular dichroism and UV/vis spectroscopies were used to determine the stepwise cooperative assembly path driven by the strongest interaction in the system; the DPP units first form disordered homoaggregates via π-stacking, followed by PDI unit association to the DPP stacks by means of triple H-bonding.

In FY14, the team also demonstrated that these DPP-PDI systems display photoinduced charge separation only upon assembly. Cyclic voltammetry (CV), UV/vis and fluorescence spectroscopy was used to investigate the ground state frontier molecular orbital (FMO) energy levels of the individual compounds and it was determined that FMOs do allow the reduction of the PDI acceptor by the photoexcited DPP donor (electron transfer), or the oxidation of the DPP donor by the photoexcited PDI acceptor (hole transfer). Variable temperature fluorescence titrations and femtosecond transient absorption spectroscopy experiments led to development of an energy diagram of the DPP-PDI assembly in toluene (see FIGURE 5). The team has successfully demonstrated that photoexcitation of donor–acceptor superstructures with visible light directs the system into a charge separated state and that cooperative noncovalent bonding and FMO levels could be synergistically designed to achieve new photophysical properties that emerge only upon assembly. Future work will continue to expand the library of donors and acceptors and also investigate the assembly of these superstructures into thin films.

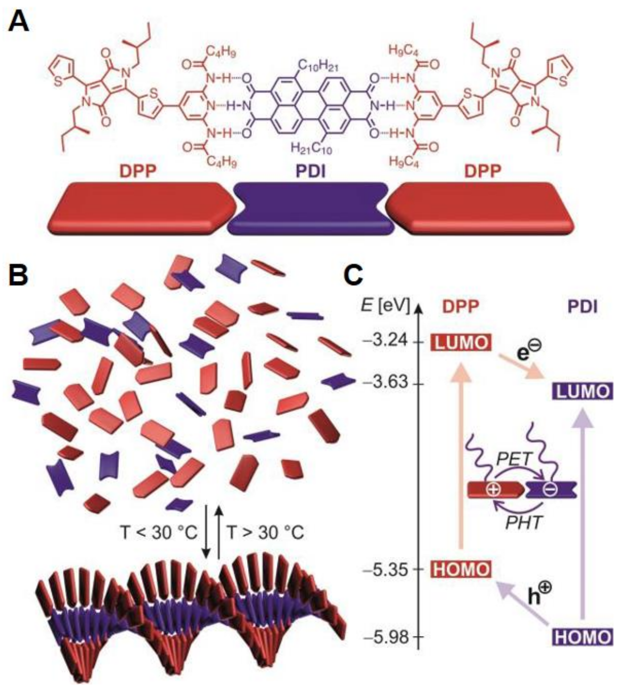

FIGURE 4

Driving supramolecular assembly of DPP and PDI; (**A**) H-bonding of DPP donor and PDI acceptor; (**B**) Heteroaggregation; (**C**) FMO scheme.

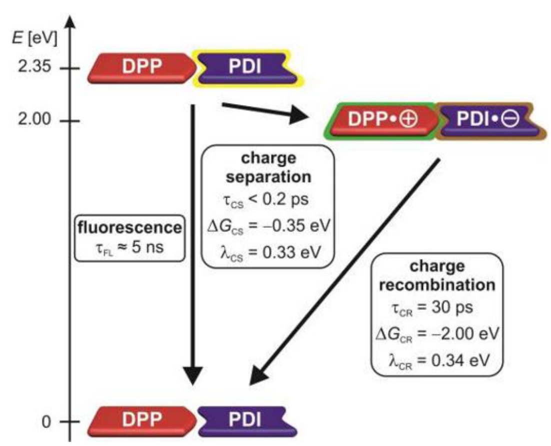

FIGURE 5

Energy diagram of a DPP-PDI assembly in toluene.

C. Probing Electrochemical Reactions at a Plasma-Liquid Interface

Professors David B. Go and David M. Bartels, University of Notre Dame, and
Professors R. Mohan Sankaran and Rohan Alkolkar, Case Western Reserve University, STIR Award

The goal of this research is to understand the nature of electron transfer from an atmospheric-pressure plasma (gas discharge) into an aqueous solution to initiate electron-driven chemistry at the plasma-liquid interface. In particular, the aim is to understand the fate of the electrons that impinge the surface – their possible solvation and their chemical reaction path. In order to probe electron behavior directly at the plasma-liquid interface, in FY14 the research team led by Notre Dame developed a novel total internal reflection absorption spectroscopy measurement (see FIGURE 6A). In short, solvated electrons absorb strongly in the red, and therefore an absorption signal at red wavelengths can be used to both confirm the existence of electrons injected from the plasma solvating in the aqueous solution and also provide cruicial insights into their behavior. Because the solvation depth of solvated electrons is ~nm, a total internal reflection geometry was required in order to enhance the signal-to-noise ratio and resolve signal intensity changes on the order of 1 part in 1 million. FIGURE 6B shows the measured absorption spectrum using a series of diode laser as well as that typically found in pulse radiolysis. As expected, there is strong absorption in the red, confirming the presence of solvated electrons. Furthermore, by analyzing the signal intensity and accounting for second order recombination of solvated electrons, we can estimate the average solvation depth to be 2.5±1.0 nm. This value is consistent with Monte Carlo predictions from the literature and suggests that these *interfacial* solvated electrons are fully solvated in the solution prior to reacting away. This is the first measurement of its kind; to date, no others have directly probed electrons at the interface between a plasma and a solution, although plasma-liquid interactions have been studied for centuries.

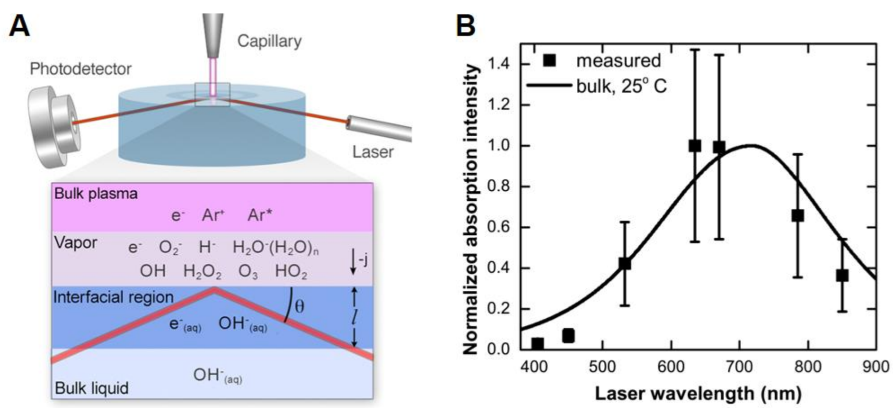

FIGURE 6

Generation and detection of solvated electrons by an atmospheric-pressure plasma. (A) Schematic of experimental apparatus for optical detection using a total internal reflection configuration. Anticipated chemical species in the different phases are also shown. (B) Measured optical absorption signal corresponding to solvated electrons measured at the plasma-solution interface by using laser diodes at different wavelengths. A Gaussian-Lorentzian bulk spectrum (solid line) measured in pulse radiolysis experiments for a temperature of 25° C is included as a guide.[2] The measurements were conducted using an argon (Ar) plasma in an Ar environment at atmospheric pressure and 0.163 M $NaClO_4$ solutions.

In order to measure the dynamics of plasma-produced solvated electrons, the research team used a series of scavengers (anion, neutral, and cation species) to quench the absorption signal (see FIGURE 7A-B). The scavengers, in this case NO_2^-, NO_3^-, H_2O_2, and H^+ (not shown), react quickly with the solvated electrons, reducing the absorbance. As expected, the signal reduction is inversely proportional to the scavenger concentration (see FIGURE 7C-D), and reaction rates extracted from these measurements are on the same order of magnitude but lower than those found in pulse radiolysis. These results, along with a measured spectrum that is blue shifted from that expected for bulk solvated electrons (see FIGURE 7B), suggest that the nature of plasma-

[2] Bartels DM, Takahashi K, Cline JA, Marin TW, Jonah CD. (2005). Pulse radiolysis of supercritical water. 3. Spectrum and thermodynamics of the hydrated electron. J. *Phys. Chem. A* 109:1299.

generated interfacial solvated electrons is distinct from electrons formed in a bulk solution using traditional radiolysis or laser photolysis techniques. Different factors, including the presence of a double layer and strong electric field and likely stratification, could all contribute to this unique behavior.

Currently, the Notre Dame team is improving the absorption spectroscopy measurement system in order to resolve differences in the plasma-liquid-produced spectrum and that for pulse radiolysis, including the sharp tail in the blue portion of the spectrum, and refine estimations of the solvation depth. Additionally, the team is studying the relationship and competition between plasma-produced solvated electrons and other dissolved plasma species such as OH•. Ongoing experiments include measuring the impact of OH• scavengers on the absorption signal as well as introducing small admixtures of O_2 into the Ar plasma to affect scavenge plasma electrons. Concurrently, the Case Western Reserve team continues to study the efficiency of plasma-initiated electrolytic reactions by comparing the amount of Ag^+ reduced in $AgNO_3$ solutions to that predicted by Faraday's law. These measurements can be used, in conjunction with reaction models, to also estimate the solvation depth and reaction rate for comparison to the absorption spectroscopy measurements.

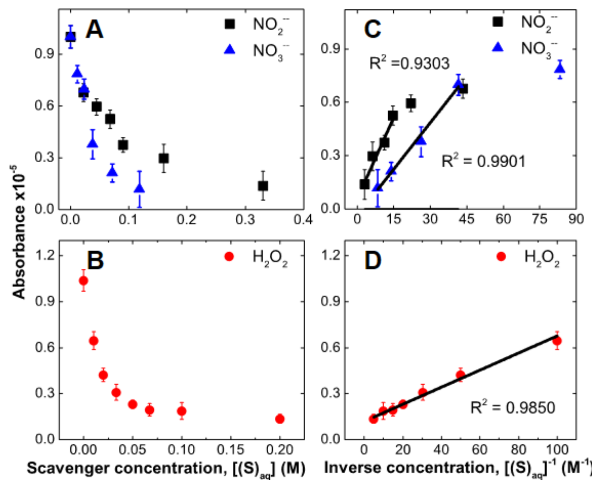

FIGURE 7

Absorbance behavior for different scavengers. (**A**) Absorbance measurements as a function of concentration $[(S)_{aq}]$ for anionic scavengers NO_2^- and NO_3^-. (**B**) Absorbance measurements for neutral scavenger H_2O_2. (**C**) Corresponding absorbance as a function of the inverse concentration $[(S)_{aq}]^{-1}$ for NO_2^- and NO_3^-, where the solid lines are linear curve fits. (**D**) Corresponding absorbance as a function of the inverse concentration $[(S)_{aq}]^{-1}$ for H_2O_2, where the solid line is a linear curve fit.

D. Post-Born-Oppenheimer Dynamics Using Isolated Attosecond Pulses

Professor Lorenz Cederbaum, University of Heidelberg, Germany, MURI award (co-PI)

Nonadiabatic effects are ubiquitous in physics, chemistry, and biology. They are strongly amplified by conical intersections (CIs), which are degeneracies between electronic states of triatomic or larger molecules. In particular, it is well-known that the Born-Oppenheimer approximation, that electron motion is completely independent of nuclear motion, is not valid at conical intersections due to the multiple electronic-state degeneracy in this region. Professor Cederbaum is a co-PI in the MURI project led by Professor Stephen Leone at the University of California - Berkeley (refer to Section II.B). As part of this MURI team, Professor Cederbaum is exploring the specific roles that CIs play in dynamical processes of energized molecules. These roles have been largely unexplored, but are thought to be highly significant for chemical reaction dynamics and photochemistry.

Recently, it was shown that CIs in molecular systems can be formed by laser light, even in diatomics. Because of the prevailing strong nonadiabatic couplings, the existence of such laser-induced conical intersections (LICIs) may considerably change the dynamical behavior of molecular systems. LICIs provide pathways for extremely fast population transfer between electronic states. This latter effect is probably the most important inherent feature of the CIs. Nevertheless, until now no one could find an unambiguous experimentally measurabe quantity that directly reflects this population transfer between electronic states for a LICI. Professor

Cederbaum's laboratory has been exploring the process whereby an ultrafast population transfer takes place between the electronic states of a diatomic molecule, providing direct evidence of the existence of the LICI. By analyzing the photodissociation process of the D_2^+ molecular ion, Professor's Cederbaum team found a robust effect in the angular distribution of the photofragments that serves as a direct signature of the LICI, providing direct evidence of its existence (see FIGURE 8)

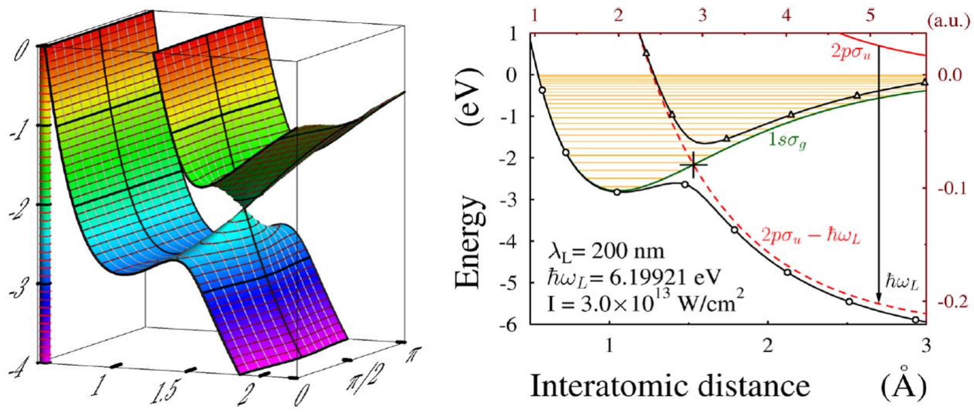

FIGURE 8

Potential energies of the D2+ molecule and the light-induced conical intersection (LICI). In the left panel are the dressed adiabatic surfaces as a function of the interatomic distance (R) and the angle (θ) between the molecular axis and the laser polarization exhibiting the LICI for a field intensity of 3×10^{13} W/cm^2. In the right panel are the diabatic energies of the ground and first excited electronic states shown by the solid green and red lines. The field dressed excited state (dashed red line) forms a LICI with the ground state, and the black lines represent a cut through the surface at θ = 0. The position of the LICI is denoted with a cross.

The PI found that the location of the intersection and the strengths of non-adiabatic couplings can be directly controlled by the laser frequency and intensity. Thus, it should be possible to control the non-adiabatic effects, such as chemical reaction dynamics, emerging from the LICIs by simply manipulating the laser characteristics during an experiment.

E. Roaming-dynamics and Electronic Relaxation Pathways in the Nitrate Radical

Professor Arthur Suits, Wayne State University, Single Investigator Award

An understanding of the elementary steps in the decomposition of energetic materials is essential to prediction of their performance, long-term stability, and sensitivity to heat and shock. A variety of sophisticated experimental approaches have thus been employed over the years for these purposes. However, even for the best available experimental and theoretical methods, gaining this fundamental understanding is quite challenging owing to the size and complexity of the molecules and the extreme conditions under which these reactions take place. The goal of this research program is to explore in detail the potentially profound impact of hitherto overlooked roaming dynamics in decomposition of energetic materials. This is achieved using a suite of powerful, complementary experimental techniques.

The nitrate radical, NO_3, is an extraordinary molecule that has fascinated and challenged chemists for many years. It possesses several low-lying electronically excited states showing complex vibronic interactions accessible via visible excitation. Its photochemistry is also quite unusual, with two dissociation channels: NO + O_2 and NO_2 + O, showing nearly the same energy threshold and accessible in the visible, giving it an important role in the atmosphere. In hindsight, the close connection between these two reaction channels may be seen as a portent of the recent recognition of the key role of roaming dynamics in this system. Roaming in the case of NO_3 is quite unusual, however. In some ways roaming in this case is analogous to nitromethane, in that it involves a roaming isomerization process; however, NO_3 clearly has been shown to involve excited electronic states (see FIGURE 9).

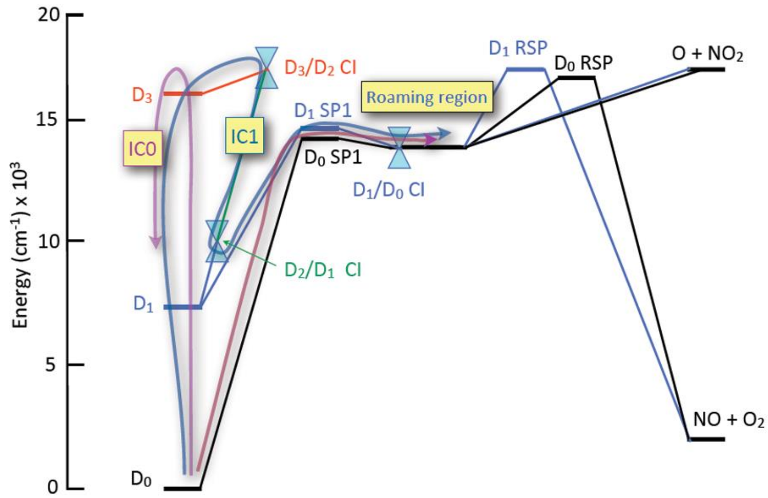

FIGURE 9

Relevant features of the potential energy surfaces of the nitrate radical.

In order to understand the complex photochemistry of NO_3 in detail, the researchers undertook experiments combining state-selected direct current (DC) slice imaging of the NO product following visible or a combination of visible and infrared excitation from a CO_2 laser, along with supplementary quasi-classical trajectory (QCT) calculations. Based on an interpretation of the results, the team concludes that following relaxation pathway is dominant: direct internal conversion (IC) from the bright state (D_3) to D_0, with D_1 subsequently accessed from the ground state, probably via mixing in the roaming region where these surfaces are strongly coupled as shown in the figure. The points in support of this view are as follows: The D_3 and D_0 surfaces possess strong vibronic coupling, directly impacting both the ground state vibrational level structure and the bright state fluorescence lifetimes, while that between the bright state D_3 and D_1 is very weak. Moreover, the fluorescence lifetimes suggest a dilution of the bright state that can only be accounted for by the ground state density of states. The fact that the translational energy distributions (not shown) are essentially identical whether electronic excitation is used with probe on a 10 ns timescale, or coupled with IR excitation 0.7 microseconds later, suggests that this relaxation is complete on the 10 ns timescale.

F. Supramolecular Polymers with Multiple Types of Binding Motifs

Professors Stuart Rowan, Case Western Reserve University and Christoph Weder, University of Fribourg, Single Investigator Award

Professors Rowan and Weder's research aims to develop multi-functional stimuli-responsive polymeric materials designed to exhibit different responses upon exposure to different stimuli and/or show emergence of new stimuli-responsive properties when exposed to multiple stimuli. One general design approach pursued by the research team involves the use of supramolecular polymers in which non-covalent interactions (π-π, metal-ligand, hydrogen-bonding) serve to assemble monomeric building blocks into polymeric structures, and also enable controlled, reversible disassembly upon application of a specific stimulus, such as a change of temperature or pH, exposure to light, or the application of a mechanical force. This allows for the design of a broad range of stimuli-responsive materials, including thermally or optically healable polymers, adhesives that permit bonding and de-bonding on demand, chemically responsive mechanically adaptive nanocomposites, or materials with built-in damage sensors.

In principle, the use of two orthogonal binding motifs, which can be disassembled by different stimuli, should permit the design of materials with multifunctional stimuli-responsive behavior, but examples of such systems are rare. In FY14, the research team demonstrated that supramolecular blends based on a poly(ethylene-*co*-butylene) core (PEB) terminated with either 2-ureido-4[1*H*]-pyrimidinone (UPy) hydrogen-bonding motifs (UPy-PEB-UPy) or 2,6-bis(1′-methylbenzimidazolyl) pyridine (Mebip) ligands coordinated to metal salts ([M(Mebip-PEB-Mebip)]X_2) display such behavior (see FIGURE 10). Through the systematic investigation of the composition-structure-property relationship, it was demonstrated that in case of the pair [Fe(Mebip-PEB-Mebip)]$(ClO_4)_2$/(UPy-PEB-UPy) the binding is truly orthogonal, and that certain characteristics of blends with appropriate composition can be selectively altered by changing the assembly of either the metal-ligand (by the addition of a competitive ligand) or the hydrogen-bonding motifs (thermally). The new materials are among the first examples of supramolecular polymer systems with orthogonal non-covalent binding motifs that display multiple stimuli-responsive behavior in the solid state.

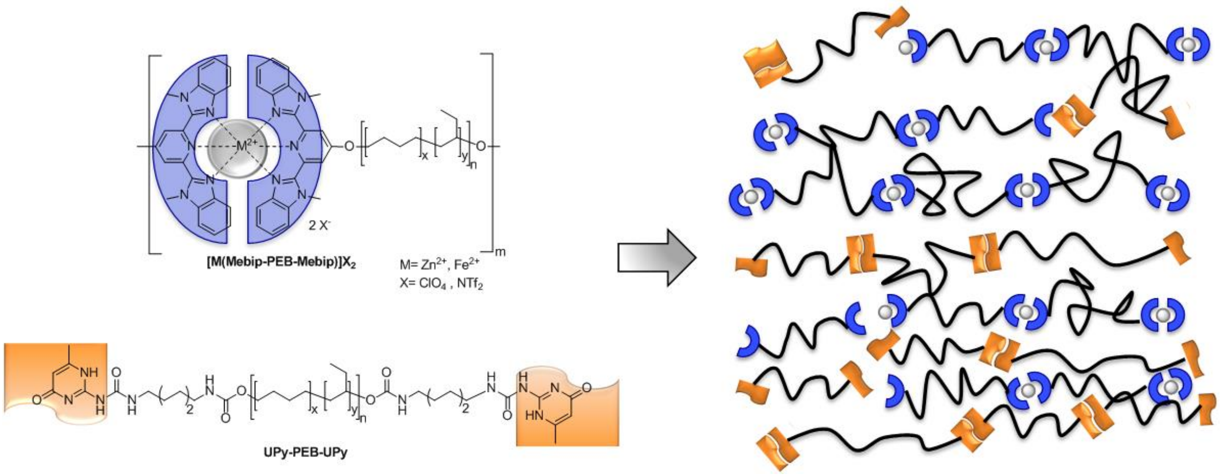

FIGURE 10

Schematic representation of supramolecular polymer blends based on poly(ethylene-*co*-butylene) telechelics and orthogonal binding motifs.

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 to external organizations and customers.

A. New multi-functional structures for sensing and decontamination

Investigator: Professor Craig Hill, Emory University, Single Investigator Award
Recipient: U.S. Army Natick Soldier Research Development and Engineering Center

The objective of this research, led by Professor Hill, is to investigate the synthesis, characterization, and chemical and physical properties of multi-functional materials that not only adsorb, but also potentially destroy or indicate the presence of a toxic chemical. Professor Hill has been focusing on designing polyoxometalate materials that can readily oxidize compounds under ambient conditions. A Cu-containing polyoxotunstate in combination with a tetrabromoferrate was found to be an effective air-based oxidation catalyst. The three-component catalyst however, is very hydrophilic and easily washes off of surfaces and fabrics. This past year, the team has focused on modification of each catalyst component to make them more hydrophobic and stable under a variety of environmental conditions (see FIGURE 11). In FY14 materials with increased hyrophobicity transferred to NSRDEC where they are immobilizing these catalysts on fabrics and testing for their ability to oxidize toxic chemicals.

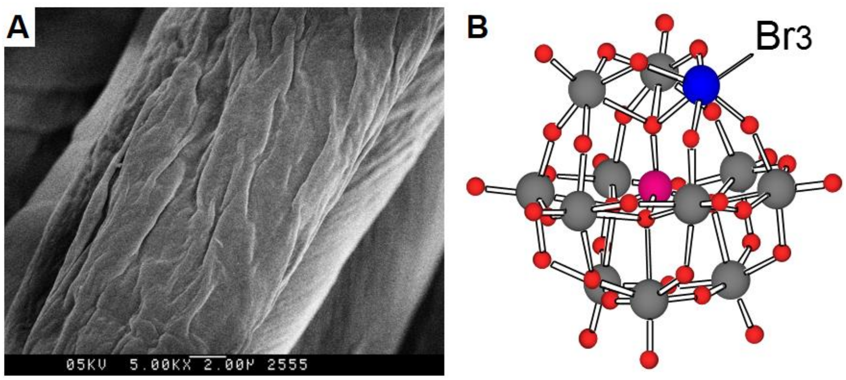

FIGURE 11

(**A**) SEM image of hydrophobically immobilized 3-component catalyst on fiber surface; (**B**) structure of $[CuPW_{11}O_{39}]^{5-}$ (POM) catalyst.

B. Describing electronic resonances in a single-reference formalism

Investigator: Professor Anna Krylov, University of Southern California, Single-Investigator Award
Recipients: Professor Richard Mabbs, St. Louis University; Professor Robert Moszynski, University of Warsaw, Poland; Professor Nimrod Moiseyev, Technion, Israel Institute of Technology

This research is pursuing electronic structure method development targeting electronic states that are metastable with respect to electron detachment and computational studies of fundamental chemical processes involving molecules and radicals in highly excited and ionized electronic states. Electronically excited molecules play a role in the initial steps of decomposition of energetic materials such as explosives that release vast amount of chemical energy in a very short time scale. In extreme energetic environments, ionized and highly excited states can also be produced giving rise to dilute detonation-generated plasmas. Thus, elucidation of elementary chemical steps in the initiation and the propagation phases of energetic material decomposition requires theoretical modeling of molecules and radicals in highly excited states that lie above the ionization threshold. Another type of metastable species, anions produced by electron attachment to neutral closed-shell molecules, is also important in plasma-like environments (electric arcs, supersonic combustion, plasma displays, extremely hot flames, lightning, polar aurorae, etc). Such metastable electronic states that lie above the ionization (or electron-detachment) continuum are called resonances. Theoretical description of resonances is exceptionally difficult, as their wave functions are not finite and, therefore, cannot be represented by expansions over gaussian basis sets. The PI has developed complex-scaled equation-of-motion coupled cluster (cs-EOM-CC) methods that allow computations of energies, properties, and lifetimes of these states. Some applications of interest include quantitative description of energetic molecules and radicals relevant to detonation of explosives. The named recipients are using the codes developed by Anna Krylov to study resonances and their phenomena in their own research projects.

C. Li_2S-Carbon Composite Technology for Li and Li Ion Batteries

Investigator: Professor Gleb Yushin, Georgia Institute of Technology
Recipient: Sila Nanotechnologies, Inc.

Professor Yushin's team recently discovered new mechanisms of stabilization of sulfur-based cathode in Lithium-Sulfur and Lithium-Lithium Sulfide cells in novel electrolyte systems, which involve in-situ formation of effective protective coatings on the cathode surface. Such coatings prevent polysulfide dissolution and, at the same time, allow rapid transport of Li ions. As a result, greatly enhanced stability and rate performance could be achieved for this high specific energy battery system (see FIGURE 12A). Professor Yushin's team also developed new routes for the low-cost bottom-up assembly of core-shell Li_2S-C composite nanoparticles (see FIGURE 12B) that allow nearly 100% capacity utilization, further enhanced stability and greatly improved rate performance. Low-cost sulfur-based cathodes not only offer an order of magnitude higher gravimetric capacity compared to traditionally used lithium metal oxide cathodes, such as lithium cobalt oxide (LCO), lithium nickel cobalt manganese oxide (NCM) and lithium nickel aluminum oxide (NCA), but additionally allow for significantly enhanced safety features. Their common limitations include rapid degradation, low capacity utilization and low rate performance. The breakthroughs in Yushin's laboratory demonstrated clear pathways to overcome these limitations and transitioned to Sila Nanotechnologies, Inc., for the commercialization of novel low cost materials for ultra-high specific energy and ultra-high energy density electrochemical energy storage technologies.

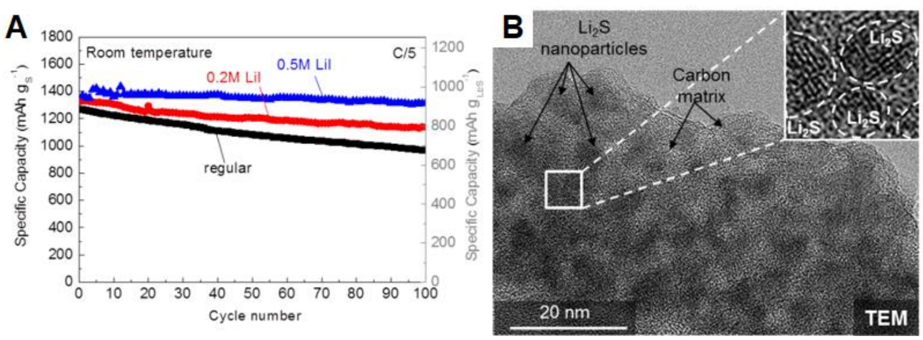

FIGURE 12

Improved S cathode technology. (A) Impact of LiI additives on the improvement of Li-Li_2S cell stability; (B) TEM micrograph showing small 5-10 nm nanoparticles of Li_2S incorporated into conductive carbon matrix.

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. Reactive Chemical Species Stabilization and Fundamental Studies of Small-Molecule Reactivity in Metal-Organic Frameworks

Professor T. David Harris, Northwestern University, YIP Award

The objective of this effort is to design and synthesize porphyrin containing Metal-Organic Frameworks (MOFs) and study their stability and reactivity in catalytic transformations, as well as their ability to stabilize small reactive molecules. This research will focus on the isolation and reactivity of iron-nitrogen multiply bonded species. MOF-545 will be used as a base scaffold material and high-valent iron-nitride species will be incorporated into the framework. Initial work in FY14 led to the synthesis and characterization of PCN-224FeO_2 which is a compound containing a five-coordinate porphyrin iron-dioxygen adduct embedded within a MOF scaffold (see FIGURE 13). This is the first structurally characterized example of any five-coordinate iron-dioxygen species.

In FY15, it is anticipated that the team will fully characterize this structure as well as other redox species to probe stability and reactivity with oxygen NO_x and CO_2. This research will provide a comprehensive understanding of the stability and reactivity of iron porphyrin containing MOFs. These multifunctional materials have potential applications for the Army in decontamination, sensing, soldier protection, and self-responding materials.

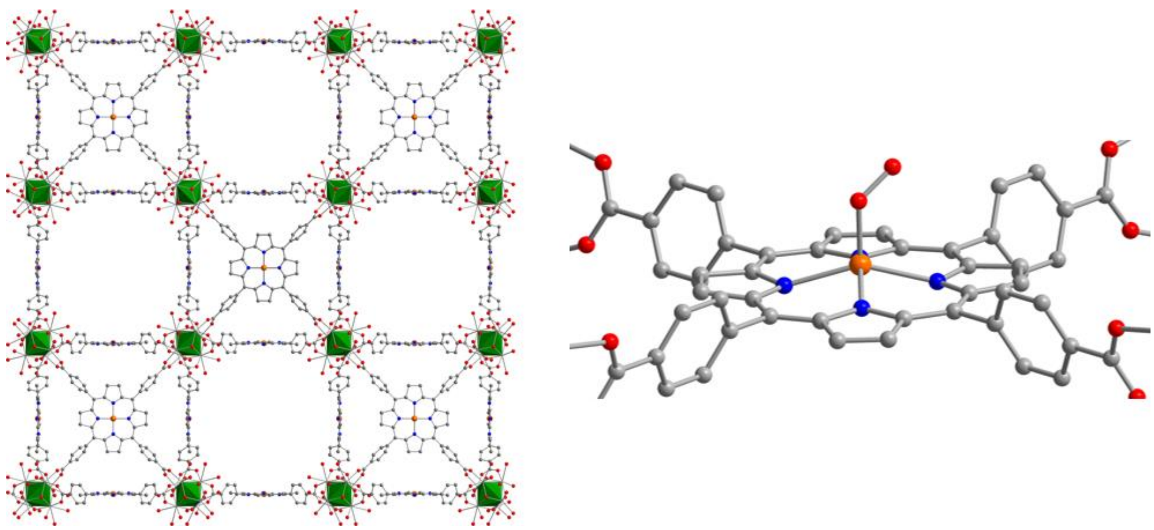

FIGURE 13

MOF Framework with PCN-224Fe (left) and crystal structure of PCN-224FeO_2 (right).

B. Chemical Transformations via Photon-induced Metal-to-molecule Electron Transfer on Metal Nanocrystal Surfaces

Professor Phillip Christopher, University of California - Riverside, YIP Award

Professor Christopher is studying photon-induced electronic transitions localized at adsorbate-metal nanoparticle interfaces and the exploitation of these events to control the outcome of selective catalytic reactions. The proposed research is intended to introduce novel selective pathways for important fuel and chemical production reactions that cannot be achieved with current classes of heterogeneous electron, photon or thermally driven catalytic processes.

In FY14, Christopher's group identified and characterized resonant electronic transitions localized at Pt-CO interfaces on small Pt nanoparticles, and showed that resonant photoexcitation of these electronic transitions allows rational control of selectivity in the preferential oxidation of CO in H_2 rich environments (see FIGURE 14). In FY15 it is expected that site-specificity and excited state dynamics of electronic transitions in the Pt-CO system will be characterized using isotopic labeling and diffuse reflectance Fourier transfer infrared spectroscopy experiments. Further, the insights will be extended to other chemical systems.

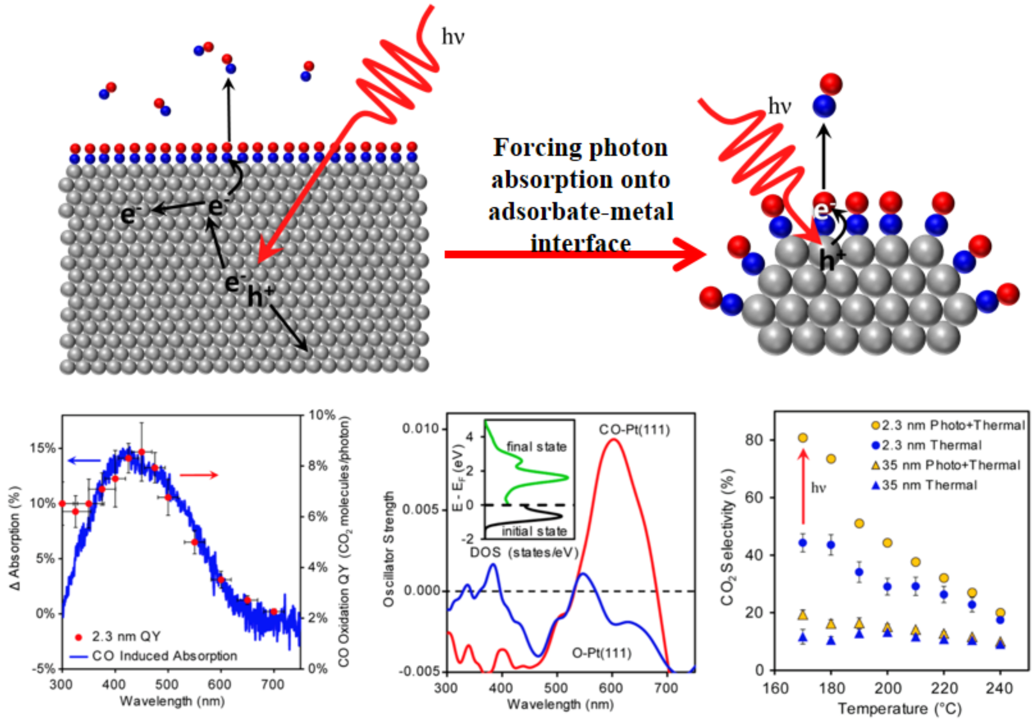

FIGURE 14

Impact of photons on metal catalysis. (Top) Schematic showing how nanostructuing of metal particles forces photon absorption to occur at surface atoms. (Bottom) UV-Vis absorption, Density Functional Theory and kinetic analysis of the impact of photon excitation on the outcome of catalytic processes occurring on metal nanocrystals.

C. Development of an Ultrafast Probe for Control of Chemical Dyanmics

Professor Wen Li, Wayne State University, Detroit, Michigan; DURIP and PECASE Awards

The goal of this research is to (i) to develop a novel time-resolved probe that will provide unprecedented new details of electronic/nuclear structure and real-time dynamics of polyatomic molecules, and (ii) to explore a new method of controlling chemical reaction using a strong mid-IR laser. It is anticipated the PI will achieve these objectives in FY15. To achieve the first objective, the PI will directly determine nuclear and electronic structure during a chemical reaction using a combination of high-order above-threshold ionization with a mid-IR laser and time-resolved photoelectron spectroscopy implemented with an extreme ultraviolet laser source. This new approach will provide a complete time-domain atomic level picture of chemical reactions as well as a direct method for mapping out multiple potential energy surfaces of polyatomic molecules, for the first time. To achieve the second objective, the PI will combine molecular axial alignment/orientation and an ultra-short strong mid-IR laser excitation to pump a large amount of kinetic energy into specific vibrational modes. In this control aspect, the PI will demonstrate a new method of achieving mode-selective chemistry using an ultra-short, intense mid-IR laser pulse. The PI has already shown theoretically that this can be achieved due to an efficient pumping of kinetic energy into specific vibrational modes when the laser intensity is much higher than that used in conventional infrared multi-photon dissociation.

D. Redox-Switchable Coordination Catalysis: An Advanced Tool for Catalyst Control and Tailored Polyolefin Synthesis

Professor Brian Long, University of Tennessee, Knoxville, Young Investigator Award

The overall objective of Professor Long's research is to develop redox-switchable olefin polymerization catalysis (RSOPC) as a cutting-edge tool for catalyst control and tailored polyolefin synthesis (see Figure 15). To accomplish this objective, the research team will develop a library of redox-active ligands and their corresponding metal complexes, examine their redox behavior and ligand non-innocence, explore the effect that ligand oxidation state has on catalytic activity and polymer branching and topology, and lastly investigate the feasibility of in situ RSOPC as a potentially pathway to unique block copolymers from a single monomer source and catalyst.

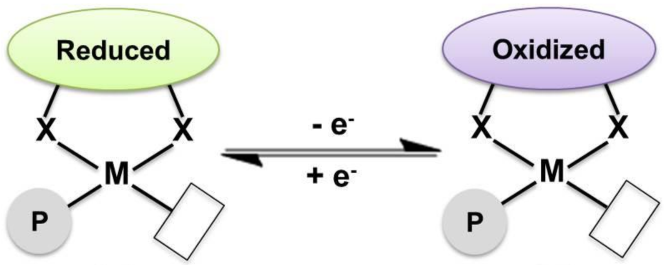

FIGURE 15

Overview of redox-switchable coordination catalysts.

In FY14, the research team established clear differentiation between reduced and oxidized states of an active olefin polymerization catalyst, and have conclusively demonstrated the ability to increase or decrease polyolefin branching content simply via changing the redox-state of our catalyst (see Figure 16). In FY15, specific research aims will be to expand their library of redox active ligands, elucidate the exact structure of reduced/oxidized catalysts, examine those catalysts for propylene and higher α-olefin polymerizations, and lastly to investigate in situ redox-switching of those olefin polymerization catalysts for the ultimate goal of polyolefin block copolymer synthesis. If successful, RSOPC will provide a substantial leap in the field of olefin polymerization by bringing a unique tool for catalyst control and advanced polymer synthesis to the field of olefin polymerization.

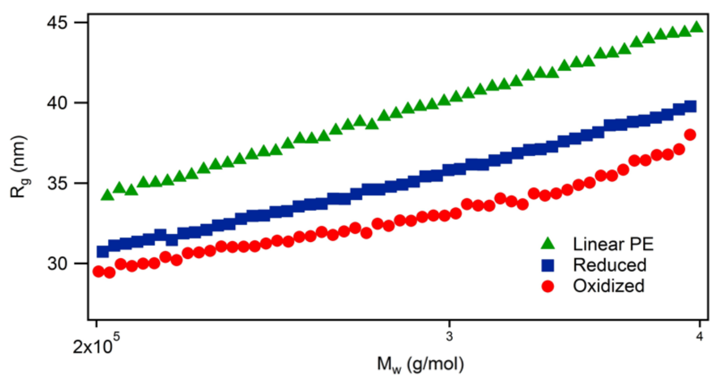

FIGURE 16

Plot of polyethylene R_g versus M_w.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Jennifer Becker
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Program Manager, Reactive Chemical Systems

Dr. Robert Mantz
Program Manager, Electrochemistry

Dr. James Parker
Program Manager, Molecular Structure and Dynamics

Dr. Dawanne Poree
Program Manager, Polymer Chemistry

B. Directorate Scientists and Technical Staff

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Director, Physical Sciences Directorate

Dr. Peter Reynolds
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Dr. Robert Kokoska
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Dr. J. Aura Gimm
Program Manager (Incoming), Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies

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International Research Program Coordinator

Mr. John McConville
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Dr. Thomas Schneider
Contract Support, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies

C. Administrative Staff

Ms. Monica Byrd-Williams
Administrative Specialist

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 2014* is to provide information on the programs and basic research supported by ARO in fiscal year 2014 (FY14), and ARO's long-term vision for transitioning 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 basic-to-applied research transitions facilitated by this Division in FY14.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of the ARO Computing Sciences Division is to provide increased performance and capability for processing signals and data, for extracting critical information and actionable intelligence, for improved decision making, and to achieve information dominance to enhance the warfighters' situation awareness. Toward this end, the Division supports research to advance the Army and nation's knowledge and understanding of the fundamental principles and techniques governing intelligent and trusted computing systems. More specifically, the Division supports basic research to establish new computing architectures and models for intelligent and trusted computing, to create novel data fusion and extraction techniques for efficient information processing, to create new capabilities in social informatics, and to build 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. In addition to advancing worldwide knowledge and understanding of computing science, the research efforts managed in the Computing Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. 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 the technology 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 Force operational goals. For this reason, computing science is a key technology underpinning future Army operations.

3. Coordination with Other Divisions and Agencies. 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 FY14, 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 processing, image understanding, video-based tracking, 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 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 also 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. Social Informatics. The goal of this Program Area is to quantify technology-based social interaction phenomena, to develop metrics for the quantified phenomena and to develop forensic and predictive analytical and computational models based on these quantifications and metrics. This new Program Area was established in late FY11. The objects of interest will generally be social phenomena (social groups/structure) and socio-cognitive phenomena (human intentions in a social context). The quantification and metrics of interest to this program are those based on domain-scientific principles of social and socio-cognitive science that are at the same time mathematically consistent and computationally feasible. Research of interest to the Program Area includes quantified, analysis-based research about technology-based social interaction phenomena in the following two Thrusts: (i) Quantification and Metrics and (ii) Analytical and Computational Models. Understanding and being able to predict technology-based social networking and social media phenomena will enhance defense in current and future asymmetric conflict, especially in the technology-based component of that defense.

The Quantification and Metrics Thrust focuses on the extraction of information from social media and requires the quantification of and metrics for these phenomena. The metrics by which one measures distance between phenomena will likely be nontraditional. Quantification and metrics need to extend to reliability and accuracy, since falsification and deception are often present at the level of the input into the social medium by a human being. Processing of soft information such as text and voice has been extensively investigated, but insufficiently in the social context that often determines meaning and that can resolve ambiguities.

The Analytical and Computational Models Thrust focuses on analytical and computational models for both forensic and predictive purposes. These models complement the qualitative models of much of sociological research, especially those in the less-investigated area of weak-tie sociology that is important for technology-based social interaction. The models are dependent on the quantification and metrics discussed above as well as on quantitatively expressed social and socio-cognitive principles. Falsification and deception may not be identifiable at the level of input information and may have to be identified by the model. The models should be embedded in applicable sociological and socio-cognitive theory and should not simply be computationally descriptive of social-media phenomena and/or be based only on analogies to physical phenomena.

C. Research Investment

The total funds managed by the ARO Computing Sciences Division for FY14 were $22.7 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY14 ARO Core (BH57) program funding allotment for this Division was $5.2 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 $5.3 million to projects managed by the Division. The Division also managed $5.5 million provided by other Army agencies and $4.5 million from other Federal agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.5 million for contracts. Finally, $0.7 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.1 million of 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 FY14 (*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 FY14 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 FY14, the Division awarded 10 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to create a framework that supports highly adaptive, stochastically-provisioned, component-based, soft real-time (SRT) applications on multi-core platforms, establish a fundamental theory of robust processing under malfunctions, inaccuracies, or unexpected situations for digital communication-based sensor networks for parameter estimation, create new methods for semantic attribute learning for robust event recognition from video data, create techniques for detection of covert groups that spread misinformation and algorithms for generating effective counter-messaging strategies that model the nonlinear dynamics of influence propagation under contradicting inputs, and to explore the use of deception and disclosures in a cyber security context to create a rigorous scientific framework to guide the development of new capabilities to defend against cyber attacks. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Derek Anderson, Mississippi State University; *Multi-Source Fusion for Explosive Hazard Detection in Forward Looking Sensors*
- Professor George Karypis, University of Minnesota - Minneapolis; *High-Performance Distributed Big Data Processing*
- Professor Baoxin Li, Arizona State University; *Learning Robust Recognition Models for Video Events Using Planning-based Semantic Feedback*
- Professor Yao Liu, University of South Florida at Tampa; *Broadband and High-power Reactive Jamming Resilient Wireless Communication*
- Professor Dinesh Manocha, University of North Carolina - Chapel Hill; *Efficient Numeric and Geometric Computations using Heterogeneous Shared Memory Architectures*
- Professor Mubarak Shah, University of Central Florida; *Visual Analytics in Multiple Camera Networks*
- Professor Venkatramanan Subrahmanian, University of Maryland - College Park; *Cybersecurity: Deception, Disclosure, and Complexity*
- Professor Katia Sycara, Carnegie Mellon University; *Content-based Group Detection in Social Networks*
- Professor Ning Xi, Michigan State University; *Compressive Feedback for Featureless Video-based Tracking Control*
- Professor Jingyi Yu, University of Delaware; *Hybrid Spectrum Face Detection and Recognition*

2. Short Term Innovative Research (STIR) Program. In FY14, the Division awarded 17 new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to create a new estimation based method for improving the quality of image reconstruction within a compressive sensing framework, create new methods for brain computer interfaces toward establishing a bio-inspired/assistant approach to extracting salient features of functional electroencephalography (EEG) data, investigate the creation, distribution, and attack patterns of attack agents in cyberspace, and to investigate and establish quantification metrics for Moving Target Defense (MTD) enabled systems to guide the development of resilient systems. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Scott Acton, University of Virginia; *Activity Detection and Retrieval for Image and Video Data with Limited Training*
- Professor Gail-Joon Ahn, Arizona State University; *Socio-metrics: Identifying Invisible Deviant Adversaries*
- Professor Ehab Al-Shaer, University of North Carolina - Charlotte; *Formal Foundations for Wireless Network Agility*
- Professor Dror Baron, North Carolina State University; *Compressive Imaging via Approximate Message Passing*
- Professor Matthew Brashears, Cornell University; *Testing the Effects of Error and Error Correction in Human Social Networks*
- Professor Jia Di, University of Arkansas; *Side-Channel-Proof Circuit Design for Hardware Security*
- Professor William Enck, North Carolina State University; *Refining Security Policy for Smartphone Applications*
- Professor Luke Gerdes, U.S. Military Academy; *Geopositional Network Discovery*
- Professor Rachel Greenstadt, Drexel University; *Stylometry of Source Code*
- Professor Qiang Ji, Rensselaer Polytechnic Institute; *Knowledge Augmented Visual Learning*
- Professor Farinaz Koushanfar, William Marsh Rice University; *Indelible Proof-of-Presence*
- Professor Richard Kozick, Bucknell University; *Localization of Gunfire from Multiple Shooters*
- Professor Juergen Pfeffer, Carnegie Mellon University; *Online Firestorms: Understanding Negative Word of Mouth Dynamics and Hate Propagation in Social Media Networks*
- Professor Asok Ray, Pennsylvania State University; *Robust Feature Extraction for Target Detection & Classification via Symbolic Dynamic Analysis*
- Professor Douglas Reeves, North Carolina State University; *Runtime Enforcement of Security Policies*
- Professor Binh Tran, The Catholic University of America; *Adaptive Training and Collective Decision Support Based on Man-machine Interface*
- Professor Sencun Zhu, Pennsylvania State University; *Toward an Evaluation Framework for Moving Target Defense Mechanisms*

3. Young Investigator Program (YIP). In FY14, the Division awarded 3 new YIP projects. These grants are driving fundamental research, such as studies to advance the state-of-the-art in visual data analysis and processing, discover novel fundamental methodologies to reveal new understanding about interactions and intentions in human centered environments, and create proactive and holistic cyber defense techniques to ensure the trustworthiness of networked systems. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor Waheed Bajwa, Rutgers, The State University of New Jersey - New Brunswick; *A Novel, Data-Adaptive Union-of-Subspaces Approach to Processing of Imaging Data*
- Professor Yun Fu, Northeastern University; *Intention Sensing through Video-based Imminent Activity Prediction*
- Professor Danfeng Yao, Virginia Polytechnic Institute & State University; *Causality-Based Traffic Reasoning for Securing Large-Scale Networks*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY14 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Institute of Electrical and Electronics Engineers (IEEE) Conference on Communications and Network Security (CNS)*; Washington, DC; 14-16 October 2013
- *Association for Computing Machinery (ACM) Conference on Computer and Communications Security (CCS)*; Berlin, Germany; 4-8 November 2013
- *Workshop on Trustworthy Hardware*; New York, NY; 13-14 November 2013
- *Fifth Institute of Electrical and Electronics Engineers (IEEE) International Workshop on Computational Advances in Multi-Sensor Adaptive Processing (CAMSAP)*; St. Martin; 15-18 December 2013
- *Cyber Warfare: Building the Scientific Foundation*; Fairfax, VA; 13-14 March 2014
- *2014 Optical Society Incubator Meeting on Implications of Compressive Sensing Concepts to Imaging Systems*; Washington, DC; 9-11 April 2014
- *35th Institute of Electrical and Electronics Engineers (IEEE) Symposium on Security and Privacy*; San Jose, CA; 18-21 May 2014
- *2014 Image Science Gordon Research Conference: Accelerating the Pace of System Design and Task-Based Evaluation*; Easton, MA; 8-13 June 2014
- *International Conference on Spectral and High Order Methods*; Salt Lake City, UT; 23-27 June 2014
- *Design for Security Workshop*; Marina del Rey, CA; 23 July 2014
- *Cyber Security: From Tactics to Strategies and Back*; Chapel Hill, NC; 23 September 2014

5. Special Programs. In FY14, 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 three 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. Principles for Robust and Resilient Tactical Mobile Ad-hoc Networking Systems (MANETs). Two MURIs in this topic area began in FY08, with one research team led by Professor Vigil Gligor at the University of Maryland and the other led by Professor Prasant Mohapatra at the University of California, Davis. The goal of these MURIs is to use insights from multiple disciplines, such as network science, engineering, mathematical science, and systems theory to develop the analytical models, tools, and mathematical representations for assessing, prescribing, analyzing, and predicting the behavior of robust and resilient mobile ad hoc networks under a total threat spectrum, and to provide security, robustness and resilience for tactical MANETs.

These MURIs focus on addressing one of the main research challenges of the Computing Sciences Division, Information and Software Assurance Program, Highly Assured Tactical Information Thrust. The research teams will investigate: (i) mathematical representations and tools for modeling and analysis of resilient and robust MANETs, (ii) theories that explain the MANET layered architecture and cross layer interaction (both intentional and unintentional), (iii) theories that elucidate the relationships and understanding of the trade-offs between fragility and robustness, (iv) interaction of networks, particularly, MANETs, low energy wireless sensor networks, and wired communications networks, and (v) design of MANET survivability algorithms and architecture, resilient management mechanisms, threat spectrum analysis for information applications on MANETs, fault tolerant and attack resilient communication protocols, survivability requirements engineering, and security and trustworthiness in MANETs.

The team led by Professor Gilgor is using a research approach based on the fundamental principles of active protocol monitoring for performance, stability and adversary handling, of employing communication channel diversity for robust end-to-end operation in the face of failures and deliberate attacks, and of exploiting cross-layer interaction for predicting the effects of performance changes caused by layer-specific failures and attacks on end-to-end MANET operation. Design and analysis techniques found in network theory, statistics, game theory, cryptography, economics and sociology, and system theory are used to develop, design and analyze models, tools, and mathematical representations for predicting performance and prescribing resilient, secure MANETs.

The team led by Professor Mohaptra is developing a cross layer architecture that provides comprehensive security and resilience. Depending on the services desired the new architecture will be able to adaptively provide the right trade-offs between performance, security and fault-resilience. The team currently undertakes three parallel but inter-coupled tasks geared towards (i) performing measurements via real deployments and enhancing understanding of layer dependencies and vulnerabilities in mobile ad hoc networks, (ii) building analytical models to characterize the behavioral nuances of these networks, and (iii) designing new cross layer protocols that protect against vulnerabilities and provide the desired robustness.

2. Cyber Situation Awareness. Two MURIs in this topic area began in FY09, with one research team led by Professor Richard Kemmerer at the University of California, Santa Barbara, and the second team led by Professor Peng Liu at the Pennsylvania State University. The goal of these projects is to explore cyber situation awareness theories and frameworks. In the long term, this research may ultimately provide more effective defense against cyber attacks, and may lead to new algorithms and systems that can assist human analysts' cognitive situation-awareness processes and decision making.

Complete situation awareness leads to effective defense and response to cyber attacks, especially those launched by adversaries with state sponsorship. The ability to extract critical information and build intelligence leads to a better capability in attack prevention, detection and response and in sustaining critical functions and services. The team is focusing research in the following key areas: (i) situation (knowledge and semantics) representation and modeling that support multi-level abstraction and transformation of data to intelligence, (ii) information fusion that can effectively combine raw and abstracted intelligence of different confidence levels to support optimal response, (iii) uncertainty management and risk mitigation through probabilistic hypotheses/reasoning and sensitivity control, which uses multi-level statistical analysis to manage incomplete and imperfect situation information, (iv) leverage cognitive science understandings to automate human analysts' cognitive situation-awareness processes (to recognize and learn about evolving situations, to create automated hypothesis generation, and to reason in both pre-attack planning and post-attack response), (v) develop a new framework unifying perception, comprehension, and projection functions and integrating situation recognition, impact assessment, trend analysis, causality analysis, and situation response together, (vi) advanced mathematic models for quantitative analysis and assessment of system assurance, and (vii) rapid repair, recovery and regeneration of critical services and functions as part of automatics response to attacks.

In this research, novel situation awareness theories and techniques are being investigated to obtain an accurate view of the available cyber-assets and to automatically determine the assets required to carry out each mission task. A proposed situation awareness framework that ties together cyber assets, cyber configuration, attack impact, threat analysis and situation visualization under cyber mission is illustrated in FIGURE 1.

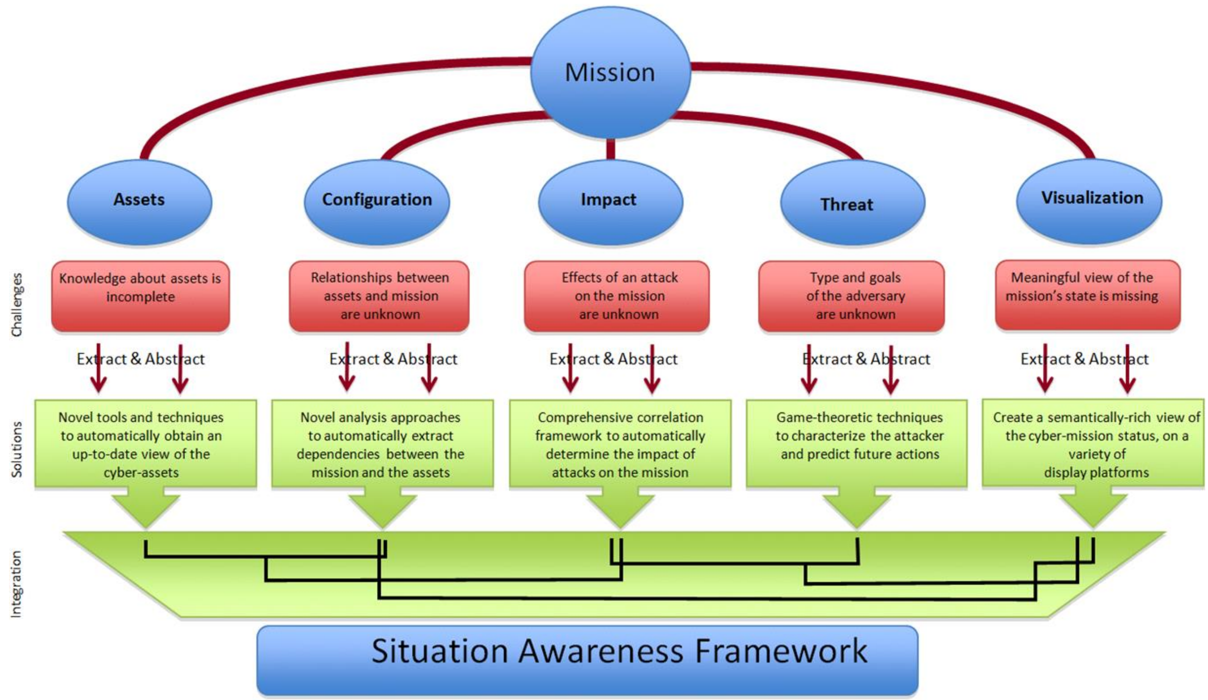

FIGURE 1

Cyber situation framework for attack analysis, prediction, and visualization. This framework incorporates cyber assets, cyber configuration, attack impact, threat analysis, and situation visualization.

3. Principles of Object and Activity Recognition Using Multi-Modal, Multi-Platform Data. This MURI began in FY09 and was awarded to a team led by Professor Richard Baraniuk at Rice University to gain a fundamental understanding of opportunistic sensing and to create a principled theory of opportunistic sensing that provides predictable, optimal performance for a range of different sensing problems through the effective utilization of the available network of resources.

This research includes four focus areas, aimed at developing a theory of sensing that can provide: (i) scalable sensor data representations based on sparsity and low dimensional manifolds that support dimensionality reduction through compressive sensing, (ii) scalable data processing for fusing image data from multiple sensors of potentially different modalities for activity detection, classification, and learning, (iii) opportunistic optimization, feedback, and navigation schemes for multiple mobile sensor platforms that adaptively acquire data from new perspectives to continuously improve sensing performance, and (iv) experimental validation on real-world inputs, such as multi-camera video, infrared, acoustic, and human language.

4. 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.

5. 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.

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

No new starts were initiated in FY14.

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 FY14, the Division managed four new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of one Phase I contract, and 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 FY14, the Division managed 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 PECASE winners for each calendar year are typically announced by the White House at the end of the fiscal year. However, the 2014 PECASE recipients had not yet been announced at the time this issue of ARO in Review was completed. 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 FY14, the Division managed seven 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. 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. Started 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 dollars per 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. Interactive and Accurate Sound Propagation in Large Complex Scenes

Professor Dinesh Manocha, University of North Carolina - Chapel Hill, Single Investigator Award and Dr. Anish Chandak, Impulsonic, Inc., STTR Award

The objective of this research is to develop new interactive algorithms for acoustic simulation for analyzing wave propagation in complex environments. This research offers fundamental scientific capabilities for solving wave/sound propagation problems in highly complex, vast domains for seismology, geophysics, meteorology, geomagnetism, urban planning, immersive training, etc. The research includes development of accurate numerical methods for the wave equation, fast solutions based on sound field decomposition or geometric propagation, and development of hybrid numeric/geometric solutions. Parallel algorithms that can exploit the parallel capabilities of current multi-core CPUs and many-core GPUs for fast computations are also being developed.

In FY14, the researchers developed a new, hybrid simulation method that couples geometric and numerical acoustic techniques to perform interactive and accurate sound propagation in complex scenes (see FIGURE 2). This is accomplished by (1) decomposing the scene into regions that are more suitable for either geometric or numerical acoustic techniques, exploiting the strengths of both, (2) ensuring the consistency and validity of the overall simulation through a novel two-way coupling between the wave-based (numeric) and ray-based (geometric) acoustic solutions based on the analytic, fundamental solution at the interface, and (3) new fast, memory-efficient interactive audio rendering techniques that only uses tens to hundreds of megabytes of memory. The method is able to handle both large indoor and outdoor scenes (similar to geometric approaches) as well as generate realistic acoustic effects (similar to numeric wave solvers), including late reverberation, high-order reflections, reverberation coloration, sound focusing, and diffraction low-pass filtering around obstructions. Furthermore, the sound field evaluation takes orders of magnitude less memory compared to state-of-the-art wave equation solvers.

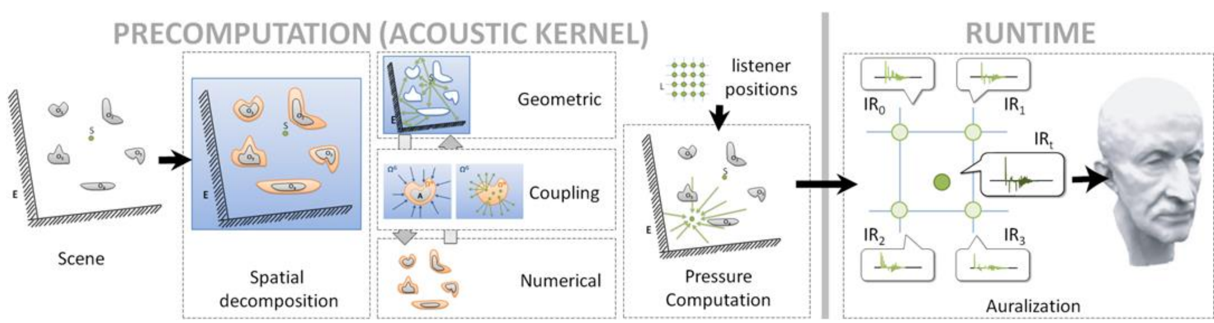

FIGURE 2

Overview of the hybrid sound propagation technique. Numerical wave simulation is used in regions with objects nearby and the geometric method for far field regions. A two-way coupling combines results from the two methods.

B. New Memory Aware Scheduling for High Performance Computing

Professors Vivek Sarkar, Dragos Sbirlea, and Zoran Budimlic, Rice University, Single Investigator Award

This research focuses on advances to the runtime environment for future systems. The goal is to integrate new runtime software with leading-edge hardware to deliver novel capabilities for monitoring and control and for interfacing with the programming environment. It is widely agreed that future supercomputer systems will be qualitatively different from current and past systems. Specifically, they will use a massive number of multi-core processors with hundreds of cores/accelerators per chip, and their performance will be driven by parallelism and constrained by energy. The performance/energy trade-offs will be further impacted by resilience because future systems will be subject to frequent faults and failures under normal operating conditions, with increased energy costs for higher reliability guarantees. There is a wide range of approaches that can be pursued in the design of advanced computing systems to explore these trade-offs.

In FY14, the researchers created a new inspector/executor based memory aware scheduling technique for future high performance computing. The inspector phase builds a dynamic computation graph without running the core computation kernels (see FIGURE 3); this graph reveals the parent-child relationship of tasks and their reader-writer relationships for data. With this knowledge, the inspector attempts to identify scheduling restrictions that lead to a bounded-memory execution. Projections indicate that the average memory per core will drop significantly in extreme scale systems. Thus, finding memory efficient schedules for parallel programs will be essential in future Army platforms.

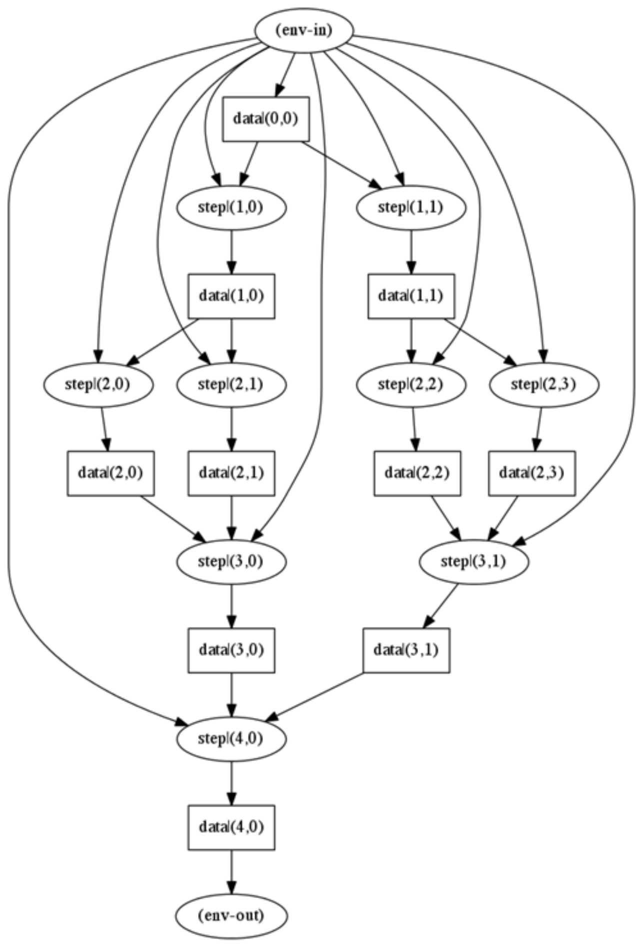

FIGURE 3

Dynamic Computation Graph created without running the computation and with automatically generated tags identifying input and output data items as well as prescribed tasks.

C. Hierarchical Models for Joint Image Segmentation and Object Recognition

Professor Alan Yuille, University of California - Los Angeles, Single Investigator Award

The objective of this research is to create novel methods and algorithms for jointly segmenting images and detecting the objects within them. The output is a labeling of all the pixels in the image. The aim of this research is to design algorithms that improve the current state of the art, while also developing a framework that can be extended to eventually create algorithms that perform as well as, or better than, human observers. The effort focuses on hierarchical compositional models where objects are compositions of parts which are in turn composed from elementary subparts. These models are learned and tested on image datasets which are benchmarked with ground-truth labels. The hierarchical models are partly inspired by knowledge of the human and mammalian visual system.

In FY14, Professor Yuille and his group at the University of California, Los Angeles, established novel integrated object detection and segmentation algorithms using bottom-up segmentation cues in combination with top-down models for objects detection. The framework allows for incorporation of part-sharing of objects, leading to exponential gains in performance speed. Research also developed models for representing articulated objects (e.g., animals and humans) in terms of parts (see FIGURE 4). Extensive experimentation demonstrated superior performance of the new algorithms for detecting and parsing objects compared to the previous state-of-the-art deformable parts models.

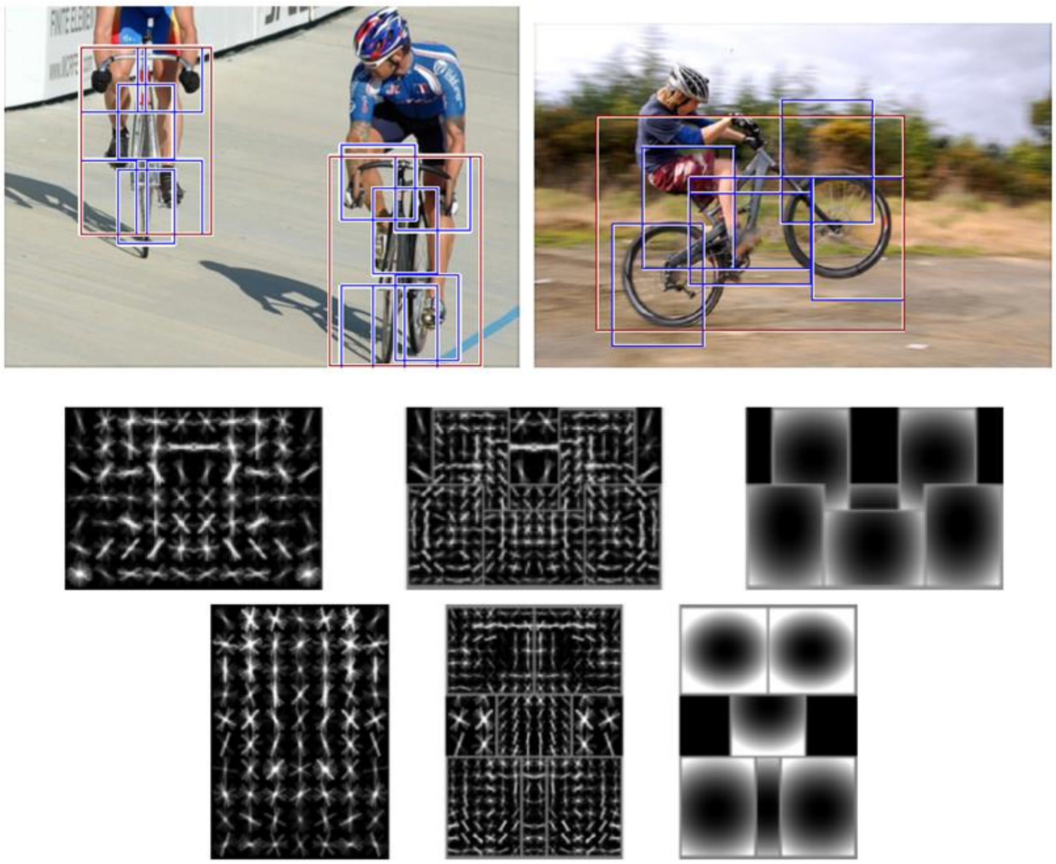

FIGURE 4

Two part based deformable models and detections obtained with a two-component bicycle model. These examples illustrate the importance of deformations mixture models. In this model the first component captures sideways views of bicycles while the second component captures frontal and near frontal views. The sideways component can deform to match a "wheelie."

D. Value Driving Information Processing and Fusion

Professor Biao Chen, Syracuse University, Single Investigator Award

The objective of this research is to create a general framework for value driven decentralized information processing that is applicable to various information value metrics. There exist diverse notions of information that can be used to quantify the value contained in given data. While they all satisfy data processing inequality and additivity under the independence assumption, difference exists that has to be addressed when developing the general framework as well as specific data processing methods that cater to distinct inference objectives. For decentralized information processing in a networked system, the value of locally processed information may not faithfully reflect its value in a global sense; data dependence is almost ubiquitous, thus decentralized processing of redundant information presents considerable challenges especially when the system is subject to various constraints. While it is known that sufficient statistics preserve information, identifying statistics that are globally sufficient in a decentralized setting is known to be a challenging problem in the presence of data dependence. Even if globally sufficient statistics can be constructed, it is known that such processing is no longer optimal when practical constraints exist at individual nodes.

In FY14, Professor Chen and his group at Syracuse University obtained conditions on the dependence structure under which globally sufficient statistics can be obtained. More significantly, when the nodes are subject to strict resource constraints, e.g., when the number of bits that can be used to represent the data is fixed, it was shown that globally sufficient statistics are not optimal in preserving the value of information. Sufficient conditions were subsequently identified that allows optimal processing at local nodes under the bandwidth constraint where the optimality refers to maximizing the eventual value of information collected at the fusion center. Among various notions of information, Wyner's common information has been much less well studied. The team undertook efforts to better understand the practical utility of Wyner's common information. A new operational metric for value of information was obtained using the Gray-Wyner's source coding network. Research also derived the explicit expression of Wyner's common information for bivariate Gaussian random variables, a problem that had remained open until recently.

E. Mining Suspicious Tiny Sub-Networks in a Massive Social Network

Professor Jiawei Han, University of Illinois - Urbana-Champaign, Single Investigator Award

The objective of this research is to create a social media data mining methodology that uncovers suspicious tiny sub-networks within massive social networks. Currently the state-of-the-art tools for exploratory network analysis such as spectral graph theory, topic models, and stochastic block models can provide insights into social behavior patterns and communities. However, these methods are not reliable in anomaly detection applications where sample size is very limited and false positive control is essential. Professor Han has developed two lines of interesting work based on a method his team developed, Dynamic Stochastic Block Model (DSBM), which overcomes the computational load present in the current state-of-the-art algorithm, probabilistic simulated annealing method. One line of this work is to mine subnetwork outliers in heterogeneous information networks. A subnetwork outlier is the kind of outlier which may not be anomalous individually but getting together as a group or a subnetwork, it will look very suspicious. For example, one person buying a pressure cooker is normal, but if you find a group of closely associated people who but a set of pressure cookers and fertilizers it could be alarming, such as the Boston Marathon bombers. Since there are exponential possibilities of combining individual nodes, the key to this work has been to develop an efficient method to mine such outlier subnetworks in large heterogeneous networks.

In FY14, the research was extended to provide a query-guided method to find user-specified outliers, such as a user input query of flights to Sochi with the subnetwork outliers as outputs (see FIGURE 5). This gives potential for researchers of other disciplines to specify what one would want to find in very large heterogeneous networks. For example, in a research network, one may like to find top-k anomalous authors who are coauthors of Professor X, but published in venues which are quite different from most of other coauthors. Professor Han has developed a query language to guide users to find such anomalies in a flexible manner. These algorithms will be applicable to the fast changing behaviors and small sample regimes that limit reliable analysis of certain social informatics data.

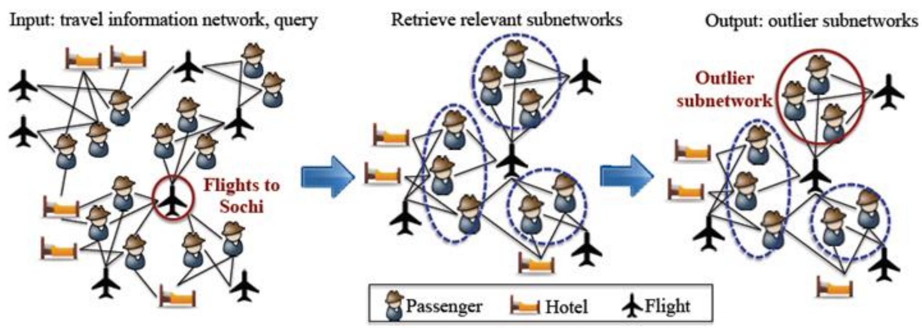

FIGURE 5

Query-guided process to identify user-specified outlier subnetworks.

F. Adaptive Manipulation of Cyber System Attack Surface

Professor Sushil Jajodia, George Mason University, MURI Award

The objective of this research is to explore the scientific foundations for adaptive cyber defense and develop a new class of technologies that will force adversaries to continually re-assess, re-engineer and re-launch their cyber attacks. Today's approach to cyber defense is governed by slow and deliberative processes such as security patch deployment, testing, episodic penetration exercises, and human-in-the-loop monitoring of security events. Adversaries can greatly benefit from this situation, and continuously and systematically probe target networks with the confidence that those networks will change slowly if at all. In fact, cyber-attacks are typically preceded by a reconnaissance phase in which adversaries aim at collecting valuable information about the target system, including network topology, service dependencies, and unpatched vulnerabilities. As most system configurations are static – hosts, networks, software, and services do not reconfigure, adapt, or regenerate except in deterministic ways to support maintenance and uptime requirements – it is only a matter of time for attackers to acquire accurate knowledge about the target system.

In order to address this important problem, in FY14, Professor Jajodia formalized the notion of cyber *system view* as follows: the attacker's view of the system as the external view and the defender's view as the internal view. A system's attack surface can then be thought of as the subset of the internal view that would be exposed to potential attackers when no deceptive strategy is adopted. Starting from these definitions, Professor Jajodia developed a principled yet practical approach to manipulate responses to attacker's probes so as to induce an external view of the system that satisfies certain desirable properties. In particular, two efficient algorithmic solutions have been created to address two different classes of problems, namely (i) inducing an external view that is at a minimum distance from the internal view while minimizing the cost for the defender, and (ii) inducing an external view that maximizes the distance from the internal one, given an upper bound on the admissible cost for the defender. Compared to traditional approaches, this novel approach presents two key advantages: (i) to introduce uncertainty for the attackers without actually changing the system's configuration, thus minimizing the overhead, and (ii) to deceive the attackers and steer them away from critical resources rather than simply introducing uncertainty and forcing them to use a random strategy.

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 to external organizations and customers.

A. Trust Integrity Measurement Architecture for Trusted Mobile Computing and Communication

Investigator: Professor Peng Ning, NC State University, MURI Award
Recipient: Samsung Research

Software and data on mobile devices (PDAs, tablets, and Smartphones) are subject to tampering and compromise. To secure mobile computing and communication, previous attempts rely on creating another layer of privileged software to monitor and check the rest of software. But pushing the trust to another layer may not always work since the added layer of software could also be subject to attacks. Trust Integrity Measurement Architecture (TIMA) solves the challenge by creating a new model of trusted code execution, which relies on 1) using hardware trust anchor (which can't be compromised) to protect the small monitoring code; 2) strong isolation from the rest of the software system, and 3) fresh code re-start for every integrity check. TIMA continuously monitors the footprint and behavior signature of every program (including the OS kernel) through attestation check on the mobile device and its associated data, and intercepts and stops any unauthorized program and data usage to defeat any potential attacks and compromises. By adopting TIMA, a mobile device can be trusted by warfighters to perform various computing and communication tasks. TIMA has been adopted by the Samsung Knox platform, with enhanced security by protecting the integrity of the entire device.

B. Quantifying the Value of Information for Situational Awareness

Investigator: Professor John Fisher, Massachusetts Institute of Technology, MURI Award
Recipient: ARL Sensors and Electron Devices Directorate (ARL-SEDD)

Value of information is critical to assessing relevance of information, prevents irrelevant information from getting processed unnecessarily, and leads to improved information processing. The objective of this research is to create a novel approach to quantify the value of information for situation awareness through distributed information gathering systems. Quantifying the value of sensing and data processing actions with regards to actionable information remains a major algorithmic and theoretical challenge. One aspect of such a problem is to (1) accurately characterize uncertainty regarding both situational awareness and the value of additional information gathering, and (2) represent the distribution of risk for decision makers. Integration of these criterion leads to intractable planning problems which scale combinatorially with the number of sensing and processing actions and exponentially over the planning time horizon. An additional challenge is to incorporate physical sensor models alongside other information sources such unstructured text. The use of graphical models provides a framework that naturally incorporates these elements and as a result of the ongoing research establishes links between information measures and bounds on risk. Specifically, optimizing informational quantities simultaneously characterizes uncertainty reduction while enabling evaluation of risk. However, computational complexity issues remain necessitating the need for computationally efficient approaches.

Professor Fisher and colleagues have, for the first time proven the conditions under which tractable greedy methods for information gathering are guaranteed to be within a factor of the optimal (though intractable) plan with regard to reducing uncertainty for situational awareness. These results have been extended to cases where the costs of various sensing actions are heterogeneous. They have established off-line algorithmic performance guarantees which are independent of the graphical structure representing the relationship between sensors and inference quantities. They have also established on-line guarantees that exploit analysis of the graphical structure to yield even tighter guarantees that narrow the gap between optimal (though intractable) and tractable greedy methods. An additional aspect of this research considers the computational complexity of computing information rewards with regards to a specific sensing plan. The complexity of computing the information reward varies with the structure of the graph in a predictable manner. Results from this effort have shown that for certain commonly used inference structures this complexity is decoupled from the information reward. The consequence is that decision makers can examine information gathering plans that have low computational complexity with high probability and that the resulting information reward will be comparable to higher complexity plans. Numerical experiments have indicated that the new approach can increase information gain by as much as 54%. Future work will address the inclusion of complex sensor models and the impact on efficient approximations to evaluating information measures on the existing performance guarantees. The research has been conducted in close coordination with the Communications and Electronics Research, Development and Engineering Center (CERDEC), the Aviation and Missile Research, Development and Engineering Center (AMRDEC) and is in the process of transitioning to ARL-SEDD for sensor network management and control.

C. 3D Modeling of Urban Sites from Point Clouds

Investigators: Professors Suay You and Ulruch Neumann, University of Southern California, Single Investigator Award

Recipient: Chevron Corporation

The objective of this research is to pursue new techniques and solutions that extend the range of urban object classes that can be rapidly processed and modeled from complex point-cloud data such as those collected from LiDAR scans. Particularly, an innovative modeling technique called "Model By Recognition" (MBR) is being pursued. The MBR is a novel alternative to traditional modeling approaches that is an entirely new and promising approach for modeling a diversity of objects with arbitrary shape, layout, and surfaces in urban environments. The research foci are the MBR framework and its key components and technical barriers including point-cloud feature detection, recognition, shape matching, and 3D model generation. The research aims to provide solutions with significant advantages over current techniques, and add important new knowledge to the science of modeling of complex data and systems.

In FY14, the initial MBR and LiDAR point cloud processing techniques were demonstrated to several government agencies and defense contractors (see FIGURE 6). Initial software transfer and evaluation for DOD and commercial applications is under discussion. The developed techniques were also presented to DoD's ISR program for wide-area surveillance applications with collected LiDAR data to be able to recognize and model targets of interest in noisy urban environments. In addition, the results transitioned to the Chevron Corporation for the development of application scenarios for the petroleum industry.

FIGURE 6

3D modeling of Atlanta, GA using point cloud data. Initial modeling results of Atlanta produced by the MBR method that includes a multitude of urban objects and structures (buildings, roads, bridges, street furniture, vehicles, and A/C units and chimneys on rooftops). The entire process was fully automatic, taking ~13 hours (original data was ~683M point clouds).

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. High Performance Distributed Big Data Processing

Professor George Karypis, University of Minnesota, Single Investigator Award

Big Data analytics represents a range of computational methods that are designed to harness the power of the vast amounts of data being generated and collected in various scientific, engineering, military, commercial, and educational domains. Experts have recognized that analyzing these vast amounts of data has the potential of generating scientific and engineering insights, enhance situational awareness and security, improve services, and produce economic value. The sheer size of the data that needs to be analyzed, and in many cases, the complexity of the analysis that needs to be performed, has made out-of-core (OoC) distributed computing approaches, which primarily store their data on disks, the preferred computational methodology. Converting existing applications to operate efficiently in an OoC distributed computing fashion is a non-trivial task as it requires a significant software re-engineering effort. Moreover, the current high-level frameworks for developing new OoC distributed computing applications, support restrictive computational models, which limit the performance that can be achieved for many classes of computations. The objective of this project is to develop methods and the associated software tools to allow message-passing distributed applications to efficiently solve problems whose data and/or memory requirements far exceed the amount of physical memory available in the underlying computer system. It is anticipated that in FY15, the message passing programming model will be extended and enhanced by introducing shared memory extensions for intra-node data sharing.

B. Semantic Descriptions Summarizing Surveillance Video with Multi-Object Tracking

Professor Alexander Hauptmann, Carnegie Mellon University, Single Investigator Award

This project is focused on generating reliable, semantically meaningful descriptions and creating summaries of key aspects of video data given inaccurate/noisy results from the component detectors. With the explosive growth of surveillance video data, automatic summarization of surveillance videos with identity aware visual diaries is an important but unaddressed problem. A visual diary consists of a series of textual descriptions with snapshots that summarize the activities of a person observed in long-term surveillance videos. As a diary is generated for each person, person-specific long-term activity statistics can also be obtained. Identities in visual diaries are critical in many applications such as assessing the health status of nursing home residents. Unlike existing methods that train activity detectors using low-level features for surveillance event detection, this research focuses on generating a summarization by tracking framework to automatically generate visual diaries. A multi-camera multi-object tracking algorithm will be constructed to perform long-term tracking. The tracking output will be utilized to detect interesting activities such as room changes, sitting down, standing up and social interactions. A visual diary for each person will be subsequently generated and important statistics such as total time spent in social interactions are automatically computed. It is anticipated that in FY15, the new algorithm will be highly scalable to process 5000 hours of a nursing home surveillance video dataset available and detect hidden trends that are impossible to detect manually.

C. Causality-Based Traffic Reasoning for Securing Large-Scale Networks

Professor Danfeng Yao, Virginia Tech University, Single Investigator Award

To support the in-depth analysis and real-time monitoring of large-scale complex systems, this research focuses on traffic causality analysis by identifying causes and consequences of anomalous events, and quantitatively assessing the real-time assurance status of large scale networks. The PI will study the network event triggering the relation discovery problem and will formalize the theoretical foundation for triggering relation discovery, as well as design, implement, and evaluate new learning and distributed discovery algorithms for its practical deployment. The work will provide new methods and tools for quantitatively analyzing the assurance of networked systems. It is anticipated that in FY15, the research team will create new capabilities of directional relations recognition, mission-specific knowledge integration in learning, and rapid distributed causal relation discovery useful for solving problems beyond the cyber security field. The new findings on ensuring system and network assurance will help the U.S. Army establish its strategic and dominant position in the cyberspace, providing practical solutions protecting the networks, hosts, and embedded systems for Army operations.

D. Testing the Effects of Error and Error Correction in Human Social Networks
Professor Matthew Brashears, Cornell University, Short Term Innovative Research Award

This research focuses on developing a promising experimental study to test the effects of error in human social networks. In many cases humans transform information as it is processed. Mistakes and transformations occur when humans encode, store and communicate information, but theories and models of diffusion of information through social networks is almost always modeled as though information is static. Misinformation and the dynamic nature of information makes models of communication much more complex than is typically captured in network models. One area of Natural Language Processing (NLP) that has begun to grapple with this topic deals with Gricean principles, which deals with the underlying, implicit rules of communication. However, fundamental principles of communication need updating with social media and network applications. The work promised to contribute to formal quantification and modeling the process by which humans introduce errors into communications. These processes are important because they lead to transformed or mutant messages that can end up competing with the initial information. It is anticipated that in FY15, this research will develop a new experimental software that examines the effects of message format, error, and error correction, in networks with more complex (i.e., non-linear) structures.

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

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B. Directorate Scientists

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Dr. Bruce West
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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 2014* is to provide information on the programs and basic research supported by ARO in fiscal year 2014 (FY14), and ARO's long-term vision for transitioning 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 basic-to-applied research transitions facilitated by this Division in FY14.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of research in the ARO Electronics Division is to gain new fundamental knowledge of phenomena that involve elementary particles and their resulting wave phenomena. More specifically, the Division supports basic research to discover and control the relationship between nanostructure and heterostructure designs and charge transport and carrier recombination dynamics, to understand and improve the 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 structures 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 require less power, interface with biological systems, and enhance the creation and processing of information, (ii) studies in electromagnetics, microwaves, and power to enable multimodal sensing for detection, identification, and discrimination of environmental elements critical to decision-makers in complex, dynamic areas, (iii) optoelectronics, which involves the use of electromagnetic (EM) radiation from radio frequency (RF) to X-ray, to interrogate, disrupt, and defeat hostile electronic and threat 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. 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.

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 FY14, 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 will involve 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, and "passive" environmental signals such as radio or TV broadcasts 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 FY14 were $22.1 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY14 ARO Core (BH57) program funding allotment for this Division was $6.3 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 $5.4 million to projects managed by the Division. The Division also managed $2.5 million of Defense Advanced Research Projects Agency (DARPA) programs. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $2.3 million for contracts. Finally, $5.6 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $1.2 million of 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 FY14 (*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 FY14 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 FY14, the Division awarded 13 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to investigate a hybrid silicon and graphene modulator approach to reduce electric power consumption and increase modulator speed for next generation data communications, charge density wave (CDW) formation in 2-dimensional (2D) mesoscopic material systems based on transition metal dichalcogenides and new emergent collective behaviors due to the confined structures, and investigate the anomalous loss resistance in field dependent (electrically tunable) high permittivity materials such as Barium Strontium Titanate (BST), exploiting recent developments in MBE and MOCVD technologies. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Ali Adibi, Georgia Tech Research Corporation; *Compact, Low-Power, and High-Speed Graphene-Based Integrated Photonic Modulator Technology*
- Professor Levon Asryan, Virginia Polytechnic Institute & State University; *Double Tunneling-Injection Quantum Dot Lasers for High-Speed Operation*
- Professor Gregory Belenky, Research Foundation of SUNY at Stony Brook University; *Novel High Power Type-I Quantum Well Cascade Diode Lasers*
- Professor M. Saiful Islam, University of California - Davis; *Heterogeneous Integrated Multispectral VIS-IR Sensors with Individually Addressable Spectrum*
- Professor Philip Kim, Harvard University; *Charge Density Wave in Mesoscopic 2-Dimansional Materials for Nanoelectronics*
- Professor Konrad Lehnert, University of Colorado - Boulder; *Wiring Quantum Networks with Mechanical Transducers*
- Professor Hooman Mohseni, Northwestern University Evanston Campus; *4pi-Steradian Curved and Lensless Imagers (4pi-SCALE)*
- Professor Tomas Palacios, Massachusetts Institute of Technology (MIT); *Terahertz Nitride Sources (TNS)*
- Professor Robert Reich, MIT Lincoln Laboratory; *Liquid Crystal Technology Support*
- Professor Zhisheng Shi, University of Oklahoma; *High Quality Self-Crystallized One-Dimensional Micro-Crystal Array For Low Loss Device Applications*

- Professor Jingming Xu, Brown University; *Infrared Rectification*
- Professor Robert York, University of California - Santa Barbara; *Investigation of RF Losses in Tunable Dielectric Devices*
- Professor Xi-Cheng Zhang, University of Rochester; *Bright THz Source and Nonlinear Field-Matter Interaction*

2. Short Term Innovative Research (STIR) Program. In FY14, the Division awarded nine new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to explore sulfur doping as an n-type (electron) dopant into InAs in order to achieve lower-loss plasmonic materials, study the basic material factors affecting the photoconductive behaviors of PbS nanocrystal quantum dots (QDs)/ZnO heterojunctions, and investigate electrically switchable terahertz metamaterials for the control of surface waves, with the potential for emission and beam forming of THz radiation from the surface of a THz circuit. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Seth Bank, University of Texas at Austin; *Sulfur Doping of InAs*
- Professor Xian-An Cao, West Virginia University Research Corporation; *Depleted Nanocrystal-Oxide Heterojunctions for High-Sensitivity Infrared Detection*
- Professor Magdy Iskander, University of Hawaii - Honolulu; *Advanced Propagation Models for Accurate and Real-time Predictions in Wireless Communication Systems*
- Professor Mercedeh Khajavikhan, University of Central Florida; *Design and Development of Electrically Pumped Coaxial Nanoscale Laser for On-chip Optical Communication*
- Professor Daniel Mittleman, William Marsh Rice University; *Switchable Terahertz Metamaterial Surface*
- Professor Daryoosh Vashaee, Oklahoma State University; *High Performance Thermoelectric Cryo-coolers based on II-VI Low Dimensional Structures*
- Professor Kevin Webb, Purdue University; *Optical Magnetism*
- Professor Peide Ye, Purdue University; Ballistic *Phosphorene Transistor*
- Professor Yong-Hang Zhang, Arizona State University; *Study of Defect Levels in Inas/Inassb Type-II Superlattice Using Pressure-Dependent Photoluminescence*

3. Young Investigator Program (YIP). In FY14, the Division awarded one new YIP project. This grant is driving fundamental research to demonstrate infrared and optical response in a carbon nanotube-oxide-metal rectenna.. The following PI and corresponding organization were recipients of the new-start YIP award.

- Professor Baratunde Cola, Georgia Tech Research Corporation; *Ultrafast Carbon Nanotube-Oxide-Metal Tunnel Diodes for Infrared and Optical Rectenna: A Study of the Limiting Resistances*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY14 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *International Symposium on the Growth of III-Nitrides (ISGN)*; Atlanta, GA; 18-22 May 2014
- *2014 Quantum Structure Infrared Photodetector (QSIP) InternationalWorkshop*; Sante Fe, NM; 29 June – 3 July 2014
- *2014 Annual Telluride Workshop for Neuromorphic Cognition Engineering*; Telluride, CO; 29 June – 19 July 2014
- *2014 Fundamental & Applied Bioelectrics Workshop*; Norfolk, VA; 14-18 July 2014
- *69th International Symposium on Molecular Spectroscopy*; Champaign, IL; 16-20 July 2014
- *2014 Lester Eastman Conference (LEC) on High Performance Devices*; Ithica, NY; 5-7 August 2014
- *International Conference on Molecular Beam Epitaxy*; Flagstaff, AZ; 7-12 September 2014
- *Conference on Infrared, Millimeter, and* Terahertz *Waves*; Tuscon, AZ; 15-19 September 2014

5. Special Programs. In FY14, 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 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 nanoelectronic and nano-optical components to biologically relevant physical properties.

In order to tap the requisite contributions from different academic disciplines (DNA chemistry, electrophysiology, nanoelectronics, 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 nanoelectronics (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 nanoelectrodes (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. Once the three test beds are functionalized, their THz spectra may provide non-trivial information about chemical composition. 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 Sun Lien Chuang 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.

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 FY14, 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 FY14, the Division managed five new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of three Phase I contracts and 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.

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 FY14, the Division managed one new ARO (Core) HBCU/MI project and seven 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 PECASE winners for each calendar year are typically announced by the White House at the end of the fiscal year. However, the 2014 PECASE recipients had not yet been announced at the time this issue of ARO in Review was completed. 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 FY14, the Division managed nine new DURIP projects, totaling $1.24 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 nine MRI programs for the High Energy Laser Joint Technology Office (HEL-JTO) in Albuquerque (managed by OSD). Six of those are new MRIs and three of those were awarded through ARO's Electronics Division (the others through Materials and Physics). The three ongoing MRIs are led by professors at the University of New Mexico, the University of Central Florida (Center for Research in Electro-Optics and Lasers), and Clemson University. These three MRIs were reviewed in FY13 and decisions were made to continue their funding for the options (years 4 and 5). Their respective foci are in three different areas: optical techniques for characterizing high power handling optical coatings and methods for improving their reliability, uses and fundamental material loss improvement and beam combining techniques with volume Bragg gratings, and solid core photonic crystal fiber laser development for larger core sizes and suppressed acoustic mode interference. The new MRIs are led by professors at Rutgers, University of Illinois, 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, reduced stimulated Brillouin scattering fiber materials, rare-earth doped GaN, polycrystalline AlN ceramic gain media, leaky wave and gas-filled hollow-core fiber lasers, and nonlinearity mitigation in fiber lasers. ARO continues to play a significant role in leading the MRI programs by organizing kickoff meetings and program reviews, particularly on the fiber laser efforts, to review progress and aid in technology transition and the development of new research programs. The ARL Computational and Information Sciences Directorate (ARL-CISD) and the ARL Sensors and Electron Devices Directorate (ARL-SEDD) participate in HEL-JTO program evaluation through annual reviews.

I. DARPA High Power Efficient and Reliable Lasers (HiPER) I Program

The objective of this program is to develop compact, efficient and bright laser-diode (LD) sources that will result in extremely light-weight and inexpensive high-energy lasers (HELs) for the U.S. military. The SRL technologies developed in the HiPER I program will increase the power-to-weight ratio of LD pumps for HELs. This program follows on the previous DARPA/ARO funded program, HiPER I. HiPER II takes the thermal modeling efforts of HiPER I and pushes the entire pump module forward to create an array of modules that will be used in the DARPA Adaptive Photonic Phased Locked Elements (APPLE) Program together with RIFL (Revolution in Fiber Lasers) Program. ARO is involved in this program by providing assistance in leveraging technical knowledge of many related JTO-HEL programs and DARPA's APPLE program. ARL-CISD is a co-PI in the new APPLE program, which uses fiber lasers to achieve beam steerable laser arrays. Integrated diode laser bars may provide further miniaturization to such systems. Progress has continued with the program in FY14, with an additional ARO managed program also under this heading to make a 1 kW or more pump module with a fiber coupling and alignment fixture for use in the DARPA EXCALIBUR fiber laser program.

J. DARPA High Power Laser Diode Facet Passivation Program

Another follow-on program to HiPER II is a result of discoveries that catastrophic optical mirror damage (or COMD) continues to plague laser bar power limits. ARO led discussions with Science Research Lab (SRL) which led to this ARO/DARPA effort as well as an ARO/DARPA SBIR. DARPA and ARO began a program to systematically study and understand the optimal facet passivation. ZnSe is known to be used in a number of laser diode commercial products, but other opportunities exist for better lattice matching and thermal expansion matching. Much of the effort is focused on using materials similar to those used in the laser itself. DoD will benefit from these studies as they help identify the best materials and processes to complete the passivation, which may lead to further improvements in power handling. Progress in the past year has been made in learning to grow the passivation materials epitaxially with further work forthcoming to characterize their performance.

K. 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 works with this program by suggesting and monitoring basic research projects with complementary goals. In FY14, the AWARE program provided funding for two university projects that fit nicely into the Electronic Sensing program area. These included projects in theory of germanium based short wave photodetectors and 4 pi steradian imaging. The 4 pi steradian imaging proposal is based on a result in the Electronics Division's single investigator program.

L. 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 works with this program by suggesting and monitoring basic research projects with complementary goals. In FY14, the LCTI-M program provided funding 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. In FY14 the performers developed a prototype camera and delivered it to the Night Vision and Electronic Sensors Directorate. ARO was the technical monitor for this project because of a previous association with an ARO MURI concerning uncooled materials.

M. 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.

N. 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.

O. 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-manages 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.

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. P-type doping of InN Nanowires

Professor Zetian Mi, McGill University, Single Investigator Award

The objective of this research is to explore the possibility of making a reliable laser on silicon – the same platform as used for most integrated circuits. Advances toward this goal have been made in this project with the first ever p-type doping of an In containing nanowire. This doping breakthrough is significant because p-type doping is critical to formation of a p-n junction required in a direct injection laser. Crystal growth of InN is being pursued in part due to its emission wavelength of 1.5 microns making it compatible with fiber optic telecommunications. Nanowires such as the ones being grown here have a strong potential as the basis for a miniature laser due to their near perfect or defect free crystalline structure – even on lattice mismatched semiconductor substrates. InN nanowires are oriented with the c-axis perpendicular to the substrate (see FIGURE 1). This makes the exposed surfaces of reduced polarity or non-polar. Polar c-plane terminations on the other hand are problematic because the internal electric field of the crystal attracts free charge which accumulates on the surface. Such charge inhibits the ability to form p-type nanowires.

In FY14 the research team was able to directly dope p-type InN nanowires with magnesium with a molecular beam epitaxy technique involving in situ deposited seeding of In which can largely eliminate undesirable impurity atoms and minimize the formation of surface defects. This self-catalytic growth of the nanowires has been shown to be substrate invariant. Thus, lasers can be grown directly onto silicon with the desired emission wavelength of 1.5 microns for high speed data communications. This research was coordinated with ARL-SEDD for potential application to silicon photonics with high performance integrated circuits with possible transition to multiple Army platforms, and also coordinated with CERDEC research in high-speed sensor read-out of focal plane arrays in night vision goggles.

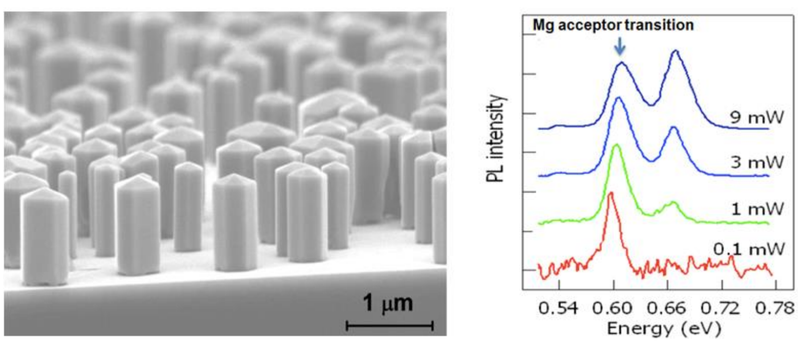

FIGURE 1

First ever p-type doping of an In containing nanowire. (Left) P-type InN nanowires grown on Silicon; (Right) Mg-acceptor related optical transition.

B. Topological Insulators for Novel Device Applications

Professor Wook Kim, North Carolina State University, Single Investigator Award

The objective 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. Utilizing the spin-momentum interlocked nature of the TI surface electronic states, the key focus is to achieve electrical control of both spin and orbital degrees of freedom for integration of (opto-)electronics and magnetics into a single nanoscale system.

In FY14, the research team has conceived and theoretically demonstrated two novel device concepts with the performances potentially far superior to the conventional counterparts. The team envisioned a structure for highly sensitive THz/far-infrared detection (see FIGURE 2). Through the coupling between top and bottom surfaces of an atomically thin TI layer as well as the exchange interaction with the proximate ferromagnet at the bottom, it was found that the optically excited carriers in the TI can be tailored to exhibit unique patterns with a strong dependence on the frequency of the incoming light as low as a few meV (i.e., in the THz frequencies). The predicted asymmetric excitation across the center of the momentum space results in the generation of robust nonzero photocurrent, leading to room-temperature detection of far-infrared/THz radiation with the advantage of low noise and fast response. The ease of frequency tuning by an external electrical bias offers an added versatility in the realistic implementation.

In a second device, the research team proposed multifunctional charge/spin current modulation on the surface of a TI in combination with a patterned layer of magnetic material (see FIGURE 3). The electronic band modification induced by the symmetry-breaking exchange interaction at the TI-magnet interface can define the path of electron propagation in analogy to the optical fiber for photons. Numerical simulations illustrated the confinement/guiding efficiency much higher than that in the waveguide formed by an electrostatic potential barrier such as p-n junctions. Further, the results indicated effective flux control and beam steering that can be realized by altering the magnetization/spin texture of the magnetic materials. This concept was extended to an FET-like transistor in combination with a magnetoelectric switching gate as shown schematically in the right figure. The preliminary results demonstrated an ultra-steep sub-threshold slope (~1 mV/decade) over a narrow bias range, highlighting the low-power advantages in the analog and digital applications.

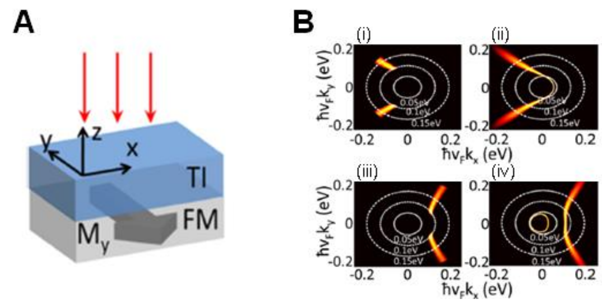

FIGURE 2

Proposed thin TI-magnet (FM) heterostructure for THz/far-IR detection. (A) schematic of the heterostructure with (B) calculated electron generation rates for the top-surface conduction band plotted in the 2D k-space. The assumed photon energies and the temperatures are: (i) 70 meV, 4 K; (ii) 70 meV, 300 K; (iii) 120 meV, 4 K; (iv) 120 meV, 300 K. The lighter color represents a stronger generation intensity.

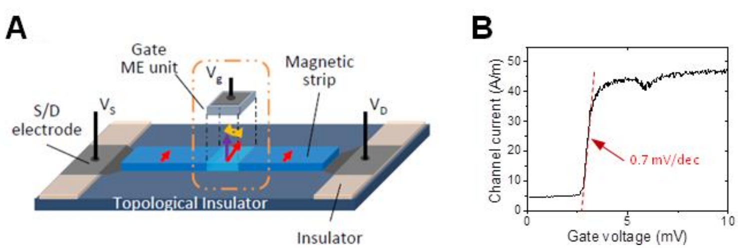

FIGURE 3

FET-like structure utilizing Dirac electron wave guiding concept and magnetoelectric (ME) gate. (A) Schematic showing the structure, where the magnetization can make a 90° rotation electrically between the in-plane and the out-of-plane orientations; (B) calculated drain current vs. gate bias. The turn-on is very abrupt with the sub-threshold slope as large as approx. 1 mV/decade over a narrow bias range.

C. Highly Efficient Terahertz Emitters and Local Oscillators Based on Nano-Plasmonic Antennas

Professor Mona Jarrahi, University of California, Los Angeles, YIP Award

The goal of this research is to exploit the localization properties of plasmonic antennas to improve the efficiency and output power of terahertz emitters based on photoconductive and photomixing techniques. In FY14, the PI successfully developed a three dimensional process for deep contact plasmonic antenna contacts integrated with a broadband terahertz antenna (see FIGURE 4). By localizing the photoelectrons generated by the optical laser pump beam, the radiation magnitude of the photoconductive emitter was improved by three orders of magnitude, experimentally demonstrating a record 7.5% optical to terahertz conversion efficiency. The technique was extended to both wideband (pulsed) and CW (single frequency) emitters. An order of magnitude enhancement in radiated power was experimentally demonstrated from a photomixer using plasmonic contact electrodes. The photoconductive emitters and photomixers were optimized for telecommunications optical wavelengths (1550 nm) to take advantage of the very high power, narrow bandwidth, wavelength tunable, compact, and cost effective optical sources commercially available. The combination of efficient terahertz emitters and photomixers provide the opportunity for a terahertz spectroscopy system with 5 orders of magnitude improvement in sensitivity.

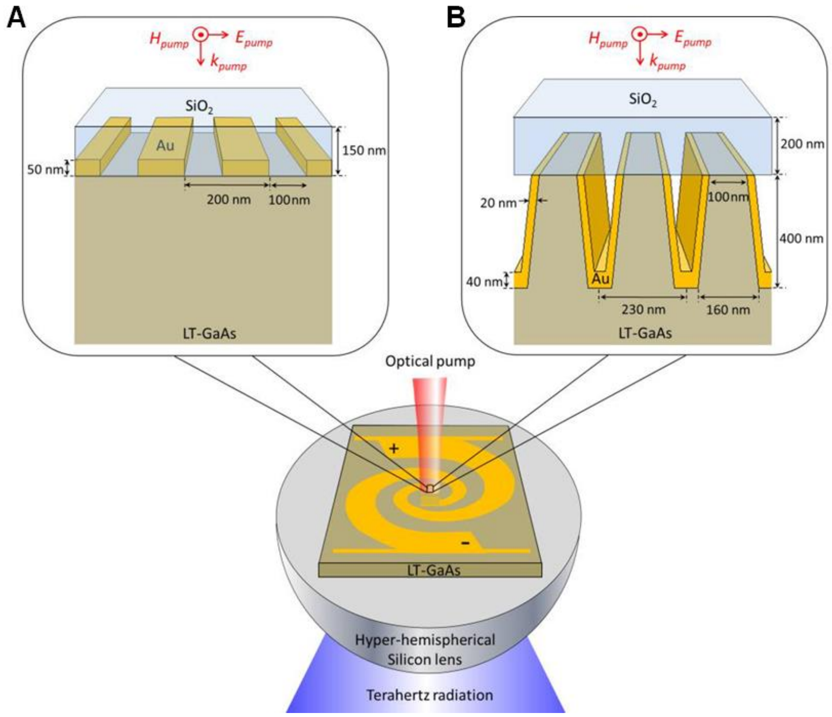

FIGURE 4

Schematic diagram of plasmonic photoconductive terahertz emitters with (A) two-dimensional plasmonic contact electrodes on the surface of the LT-GaAs substrate, (B) three-dimensional plasmonic contact electrodes embedded inside the LT-GaAs substrate.

D. Development of the III-V Barrier Photo Detector Heterostructures

Professor Gregory Belenky, State University of New York - Stony Brook , Single Investigator Award

The objective of this research is to employ metamorphic epitaxy to obtain unstrained unrelaxed layers of InAsSb and increase the bandgap beyond 10 microns with excellent carrier recombination and transport properties. Band bowing in the InAsSb material system creates a bandgap wavelength greater than 10 microns for the proper As/Sb ratio. However, it has been difficult to grow unstrained samples and the bandgap has been limited to around 5 microns. By use of compositional grading, researchers at SUNY - Stony Brook have grown unstrained samples that exhibit photoluminescence up t o12.4 microns (see FIGURE 5). Since InAsSb is a direct bandgap system, this could enable a simple bulk material for infrared detection in the 10 micron band. This should be just as sensitive as HgCdTe, but in a III-V material system, which is more robust, less expensive, and would also be simpler to fabricate than other III-V detectors that require superlattices or quantum dots.

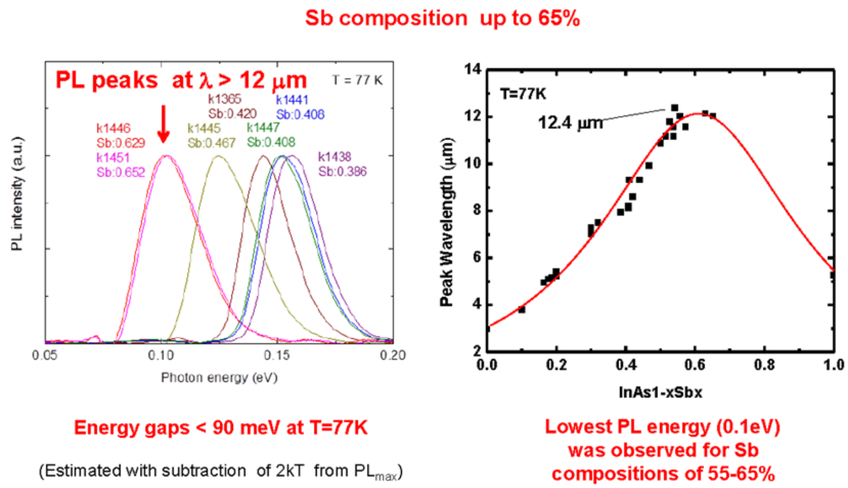

FIGURE 5

InAsSb PL peak energy at T = 77K. (Left) PL intensity for different Sb composition; (Right) PL peak wavelength versus Sb composition.

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 to external organizations and customers.

A. "Lithographic" Vertical Cavity Surface Emitting Laser Arrays

Investigator: Professor Dennis Deppe, University of Central Florida, Single Investigator Award
Recipient: Lasertel, Inc

Research on vertical cavity surface emitting lasers (or VCSELs) based on (In, Al, Ga)As semiconductor alloys has resulted in strong performance and reliability enhancements that have taken the attention of industry. The pioneering work of Professor Dennis Deppe has progressed based on investigating one of the basic building blocks of commercial VCSEL processes known as the "native oxide". Lasertel, Inc. noticed that the strong improvement in both the power output and the reliability of the VCSELs were significant and began collaborating thru a licensing agreement to transition some of the technology toward their VCSEL array products. Wet oxidation of the AlAs layer used to form this oxide, AlxOy, is a controllable and desirable process to form a current aperture that direct carriers into the active light emitting region of a VCSEL. The process is well known and regarded as foundational to commercial VCSELs today due to the ease of its inclusion in a fabrication process and its usefulness as both a current aperture and partially as a guidance mechanism. However, the need for it has been obviated by a new "lithographic" approach used by Professor Deppe; whereby, his "phase-shifting mesa" isolates the laser mode to a central region where the charge carriers recombine much faster due to the stimulated emission process caused in the laser cavity (see FIGURE 6).

The result of removing the oxide has been tremendous on a few counts: (i) the oxide served as a large thermal barrier to heat dissipation and increased device temperature dramatically causing gain saturation at lower temperatures than necessary and reduced reliability (ii) the wet oxidation process to form the VCSELs obviated the possible use of AlAs for the distributed Bragg reflectors, known as "DBRs" on either side of the active region. Such DBRs consist of 20-30 or so pairs of AlAs/GaAs quarter-wavelength layers that create a high quality factor laser cavity important for low-threshold current lasing. By eliminating the wet oxidation process from the VCSEL fabrication, Professor Deppe's VCSELs incorporate AlAs for the DBRs and improve thermal conductivity of the top and bottom mirrors surrounding the light emitting region dramatically. AlGaAs alloys needed for "oxide-VCSELs" have a significantly reduced thermal conductivity compared with binary AlAs compounds. The use of this new process by Lasertel, Inc. has allowed their arrays to be used at much high powers over significantly longer periods of time without power degradation.

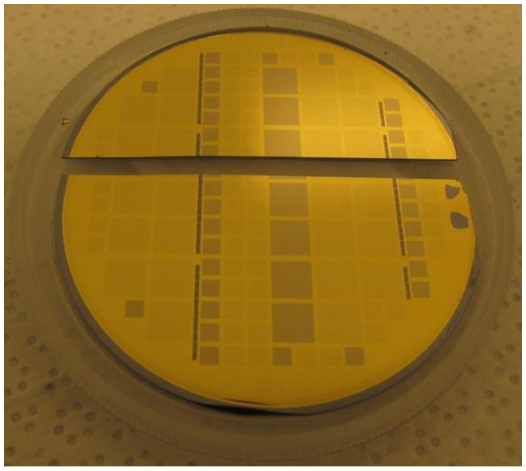

FIGURE 6
Metallized VCSEL epilayers. The epilayers contain 40,000 VCSELs in a 0.5 cm x 0.5 cm array

B. Advanced Microscopy and Analytical Studies for Hg-based Infrared Detector Materials and Substrates
Investigator: Professor David Smith, Arizona State University, Single Investigator Award
Recipients: ARL-SEDD, CERDEC

HgCdTe-based devices are the basis of the Army's premier infrared (IR) sensors. However, the current detector arrays are grown on CdZnTe substrates which are expensive and limited in size. The next generation IR detectors need to be larger for improved resolution. They will most likely be grown on silicon which has a large lattice mismatch with HgCdTe which leads to deleterious defects. The work at Arizona State is using advanced microscopy to determine the microstructure of mercury based materials on different substrates as a function of growth and annealing treatment and create possible strategies for significant reduction of growth defects. This work has transitioned to a joint project with researchers at ARL-SEDD and CERDEC. Representative samples of annealed ZnTe(211)B/ Si(211) composite substrates were examined using both imaging and analytical techniques and correlations between the microstructure of the ZnTe layers with nucleation and especially growth temperature as well as geometrical uniformity and chemical composition of the top surface are being developed (see FIGURE 7). Initial observations show high densities of short {111}-type stacking faults close to the arsenic passivated Si surfaces, with a marked drop-off in dislocation density in the epilayer moving away from the substrate. This work will likely provide significant insights into the relative importance of the different growth parameters on overall material quality which should lead to a reduction of dislocation densities and surface currents and thereby to improved HgCdTe-based detectors and devices.

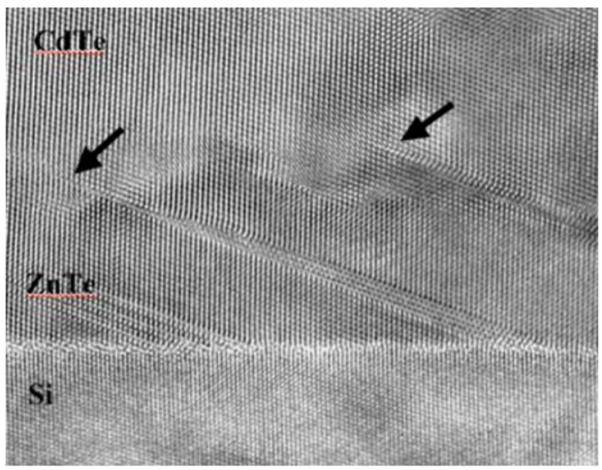

FIGURE 7

Cross-section electron micrograph showing CdTe(211)/ZnTe/Si(211) interface

C. Electromagnetic Induction and Ground Penetrating Radar Signal Processing Algorithms
Investigator: Professor Waymond Scott, Georgia Institute of Technology, Single Investigator Award
Recipients: CERDEC, NiiTek, Inc., Minelab, L3 Cyterra Corp.

The goal of this research is to explore new concepts for electromagnetic induction (EMI) sensors and ground penetrating radar (GPR) to improve their sensitivity to detect landmines and to discriminate targets from clutter. The PI has extensively modeled and measured electromagnetic target signatures for landmines and the major effect of different soil types on the signature of the buried targets. Traditional methods of exploiting target signature information, such as dictionary matching, and of exploiting the motion of the sensor, such as synthetic aperture radar, are extremely computationally intense, both in processing time and in required computer memory. In the case of landmine detection the computationally complexity renders real time processing to exploit these techniques impossible. Professor Scott has shown that the exploitation of the relaxation frequencies of the target can reduce the processing time and required memory for EMI by more than two orders of magnitude. He has developed an adaptive filtering algorithm which allows the technique to combine multiple measurements of the target. And by using a tensor representation, allowing the continuous approximation of some of the target parameters, the dictionary size can be reduced by as much as six orders of magnitude. For GPR, he has shown that structuring the dictionary information to exploit translational invariance of the target signature can reduce the dictionary storage by several orders of magnitude and that the use of the fast fourier transform provides significant further reduction in processing time, rendering the dictionary matching technique viable for previously impossible problems. Further improvements in processing and storage space have been demonstrated using compressive sensing approaches. The PI has improved the design of EMI sensors by improving shielding to improve accuracy, by improving the preamplifier to increase sensitivity, and by structuring the drive signal to the coil and by exploiting switched amplifiers to increase efficiency. He has developed a new GPR antenna structure (see FIGURE 8) which allows simultaneous emission and measurement of dual circular polarizations, in order to exploit symmetry features of targets and clutter.

The PI has transitioned a prototype EMI sensor, with processing algorithms, to CERDEC for field testing. He has worked with CERDEC to measure and evaluate target signatures and the effects of soil on target signatures. He serves on a team at CERDEC to evaluate Army EMI sensor development. He is working on a team with NiiTek, Inc, and Minelab to develop an improved combined EMI/GPR handheld landmine detector. He worked with L3 Cyterra to integrate his broadband EMI sensor concept into the Mini-H handheld landmine detection system. He has also worked with NiiTek to integrate his broadband EMI sensor array into the Autonomous Mine Detection Sensor (AMDS) program.

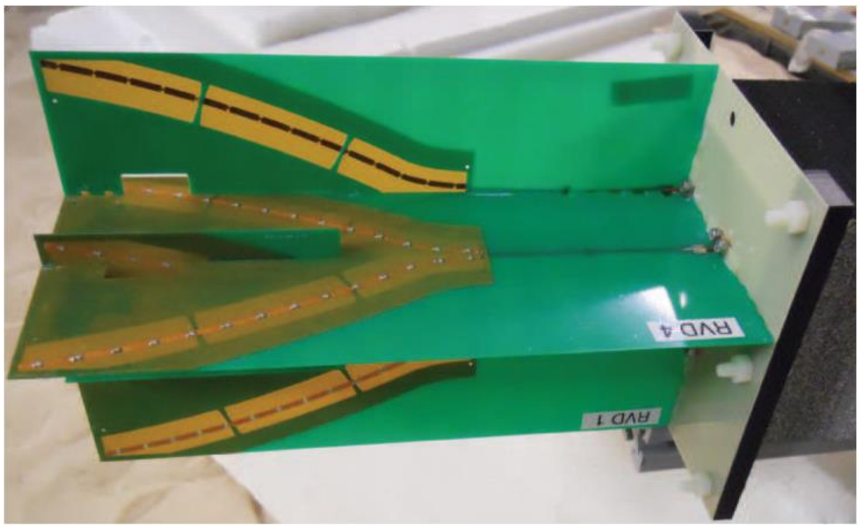

FIGURE 8

Resistive vee dipole based circularly polarized antenna. This new GPR antenna structure allows simultaneous emission and measurement of dual circular polarizations, in order to exploit symmetry features of targets and clutter.

D. 100 nm Pitch 1-Dimensional DNA Origami Arrays as Programmable Substrates for Sensing

Investigators: Professor Michael Norton, Marshall University, Single Investigator Award
Recipients: Parabon NanoLabs, Inc.

This goal of this research is to develop methods for arrangement of individual DNA origami constructs into finite linear arrays (see FIGURE 9). An important challenge in lithography is the arrangement of soft materials with high precision, stoichiometry and orientation at the ~ 3nm scale. The advent of DNA based constructs has provided one of the very few mechanisms to organize species such as proteins, molecules, nanoparticles and smaller nanostructures in close proximity to each other, enabling synergies through combining the properties of these materials. However these DNA based constructs have, for the majority, been single isolated structures. While such a format has utility for basic research, application as a commercial product will require redundancy because multiple copies of any single molecule device will be necessary for production of reliable, commercially viable sensing applications.

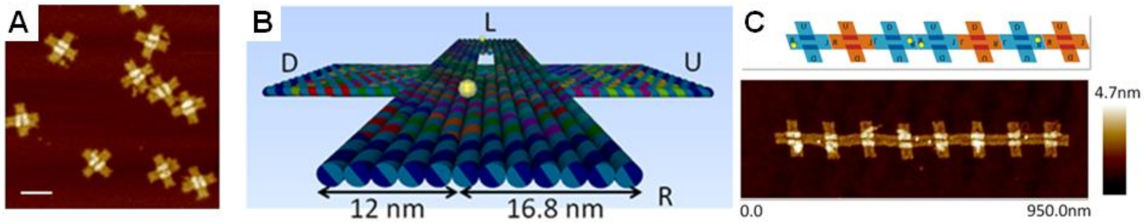

FIGURE 9

Individual DNA origami constructs arranged into finite linear arrays. (A) Atomic Force Micrograph (AFM) of individual DNA Origami constructs. White scale bar = 100nm. (B) Diagram presenting orientational information (Left, Right, Up and Down), dimensional information (nanometer scale) and location of single protein binding site (yellow dot) for the "Blue" construct component. (C) Top: Schematic view of organization of individual origami constructs in finite linear array, protein capture sites denoted as yellow dots; Bottom: AFM image of example linear array, with single captured protein molecules observable as "white dots".

Professor Norton's laboratory has successfully developed a method to construct eight individual origami blocks in a finite array (see FIGURE 9c) that provide a high level of redundancy, with the potential for on the order of 1200 addressable sensing sites. Although redundancy is important, the ability to multiplex within an array (having multiple subsets of sites within an array) is anticipated to be of importance for future sensing of molecular and biological species of interest. Although not apparent in the atomic force micrograph of FIGURE 9c, the constructs designated with Orange and Blue coloring in the diagram offer entirely different sets of potential sensing sites (~150 sites per component construct). Examples of single protein capture location (the model protein Streptavidin) are distinguishable as white dots in FIGURE 9c and only appear on the right (R) arms of the "Blue" subset of constructs. These substrates transitioned to industry and are currently being developed as substrates for sensors for chemical and biological species of interest though a joint development program with Parabon NanoLabs, Inc. Parabon NanoLabs is a start-up company with two locations, a research laboratory in Huntington, WV, in close proximity to Marshall University and a corporate office/software development arm in Reston, VA. The company was founded in March of 2008, with the mission to create breakthrough products using DNA. The new arrays contribute to the development of nanoscale sensors and related materials are anticipated to be integral parts of sensing products, addressing worldwide demand for robust, ultraminiaturized security devices for species of interest.

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. Depleted Nanocrystal-Oxide Heterojunctions

Professor Xian-An Cao, West Virginia University, STIR Award

The objective of this research is to examine the basic material factors affecting the photoconductive behaviors of nanocrystal quantum dots (QDs)/ZnO heterojunctions and explore their applicability for optoelectronic applications, including high-sensitivity IR photodetection. QDs possess many attributes that are advantageous to the development of high-quality optoelectronic devices: (i) their band gaps can be easily tuned through the size and/or composition variations to operate in different wavelength ranges; (ii) their large absorption cross-sections arising from quantum confinement effects enable more efficient light absorption than bulk materials; (iii) their solution processability at low processing temperatures provides a means for low-cost device production; and (iv) their compatibility with different substrates facilitates integration with different electronics. It is anticipated that in FY15 monodispersed and well-defined colloidal nanocrystal QDs of lead sulfides (PbS) will be spin coated on an insulting substrate and processed for photoconductive measurements (see FIGURE 10). A thin layer of ZnO will be incorporated to aid charge transport and noise suppression without decreasing gain. The photoconductive behaviors of the heterojunction will be studied in detail and their correlation with the material properties will be investigated. The proposed photoconductor is expected to have overall sensitivity well exceeding that of previously-developed QD-based photodetectors ($D^*{\sim}10^{13}$ Jones).

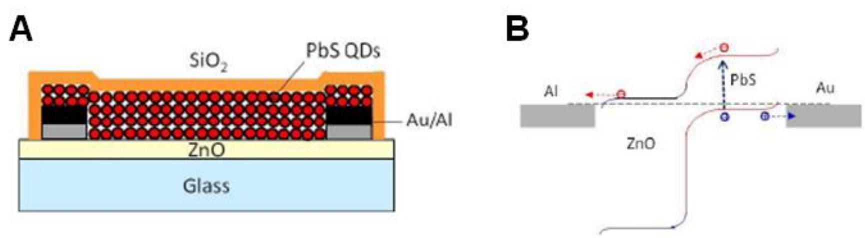

FIGURE 10

Monodispersed colloidal nanocrystal QDs of lead sulfides spin coated on an insulting substrate. (**A**) Schematic cross section of the proposed PbS QDs/ZnO photoconductor. (**B**) Energy level alignments at the Al/ZnO /PbS QDs (~4 nm in dia.)/Au interfaces.

B. Co-axial nanolasers

Professor Mercedeh Khajavikhan, University of Central Florida, STIR Award

Researchers the University of Central Florida's Center for Research in Electro-Optics and Lasers (CREOL) are pursuing a new type of nanolaser based on preliminary work completed at the University of California at San Diego under DARPA NACHOS program. It is anticipated that in FY15, the research team will produce the first electrically injected co-axial nanolaser that builds on optical pumping demonstrated by Professor Shaya Fainman's group at UCSD (former advisor of Prof. Khajavikhan). Such an advancement is of high interest due to the potential size miniaturization and high efficiency of the laser. Co-axial "donut" modes are easily scaled down in diameter and produced in a straight forward design process via access to the p and n doped regions from the inner and outer metallic conductors of the coaxial geometry (see FIGURE 11). Concern has been raised though about issues related to absorption loss in the metal, necessitating a dielectric buffer layer to reduce inefficiencies. Such optimization in design has already been investigated, and a key factor in the design is selection of the best dielectric for thermal conduction. Accurate deposition of the dielectric is a key issue, as well, in terms of thickness and refractive index. Other considerations which will be studied include coupling of the output to an output waveguide to maximize efficiency and bandwidth (if modulated output is to be used).

Once electrically injected lasing is achieved such coupling experiments can proceed and issues related to laser modulation bandwidth, switching energy, and minimum diameter can be explored.

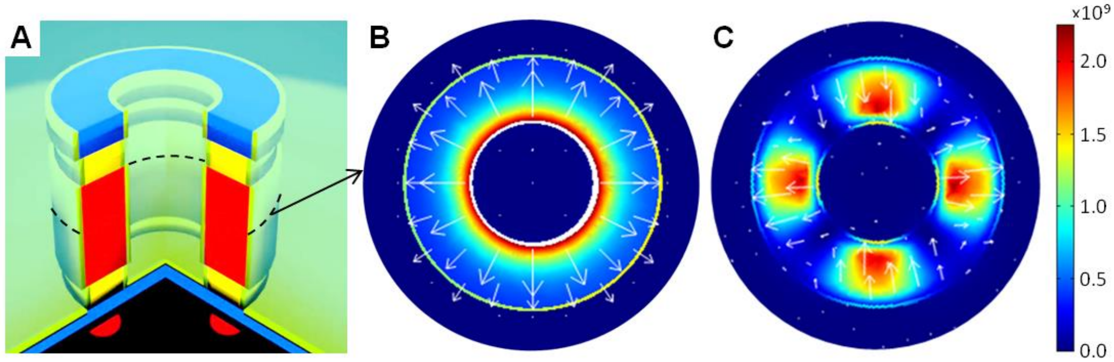

FIGURE 11

Electrically injected co-axial nanolaser that builds on prior optical pumping demonstrations. (**A**) Schematic of an electrically pumped coaxial nanolaser (**B**) Fundamental TEM mode (**C**) Higher order mode

C. Guiding High Power Laser Energy and Electrical Discharges using Femtosecond Optical Laser Pulses and Filaments

Professor Howard Milchberg, University of Maryland, College Park, Single Investigator Award

The objective of this research is to leverage the efficient and spatially extended nonlinear absorption of filamenting femtosecond laser pulses to produce extremely long lasting atmospheric refractive index structures. The PI has shown that even though the femtosecond laser generated filament lasts only nanoseconds, it creates a gas density "hole" that lasts milliseconds and that the temperature gradient driving the gas density hole can be caused or enhanced by sequences of laser pulses timed to quantum rotational revivals (see FIGURE 12). It is anticipated that in FY15, the research team will demonstrate arrays of filaments and thermal depressions which will guide pulsed and CW laser energy and electrical discharges over distances up to 50 M, with the potential for much longer distances.

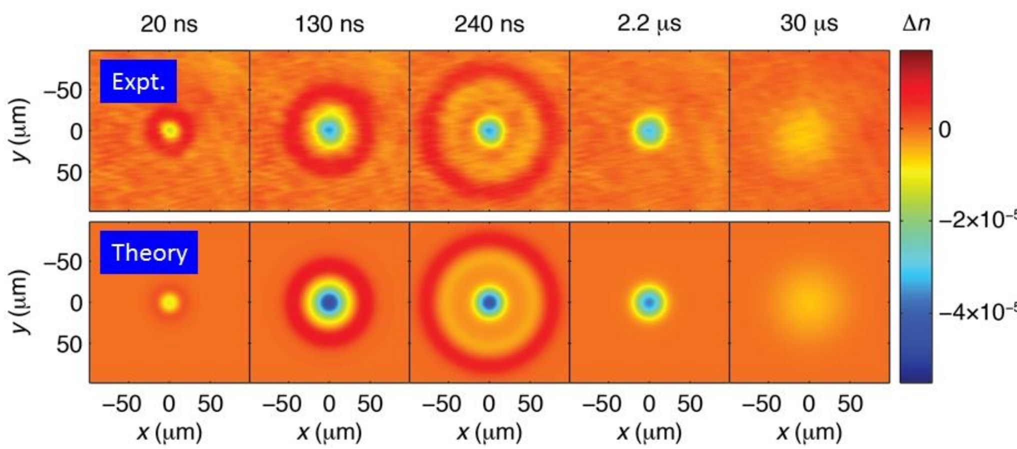

FIGURE 12

Experiment (interferometry) and simulation of nanosecond through microsecond evolution of a short filament-induced air hydrodynamic response. By 300ns, the single cycle acoustic wave is seen leaving the filament vicinity, and by ~ 1 µs, a density hole is left, which dissipates by thermal diffusion over milliseconds.

D. Charge Density Waves in Mesoscopic 2D Materials for Nanoelectronics

Professor Philip Kim, Harvard University, Single Investigator Award

The objective of this research is to investigate novel electric transport phenomena in mesocopic charge density wave (CDW) systems in coordination with nanofabrication and atomic scale resolution imaging based on transmission electron microscopy (TEM). The metallic transition metal dichalcogenides (TMDCs), such as TaS_2 and $TaSe_2$ have been important materials platform to realize robust 2D CDWs formation. The team has developed a fabrication method of encapsulated 2D CDW in the hBN layers in order to protect the surface of atomically thin TMDC materials from potential chemical reaction with the environment. The CDW structural phase has been associated with the observed variation of the phase transition as the thickness of the sample reduced (see FIGURE 13).

It is anticipated that in FY15, the research team will summarize this initial phase results in order to understand the commensuration and incommensuration phase transition in the presence of quantum fluctuation due to the reduced dimensionality and increased effect of the disorders. The team is also planning to expand their efforts to investigate the mesoscopic CDW system by creating mesoscopic scale structures to provide artificial pinning centers for discomensuration lines, which are to be believed the key element of C-IC phase transition. The researchers aim to create a switching devices based on such a controlled and engineered CDW domain wall pinning.

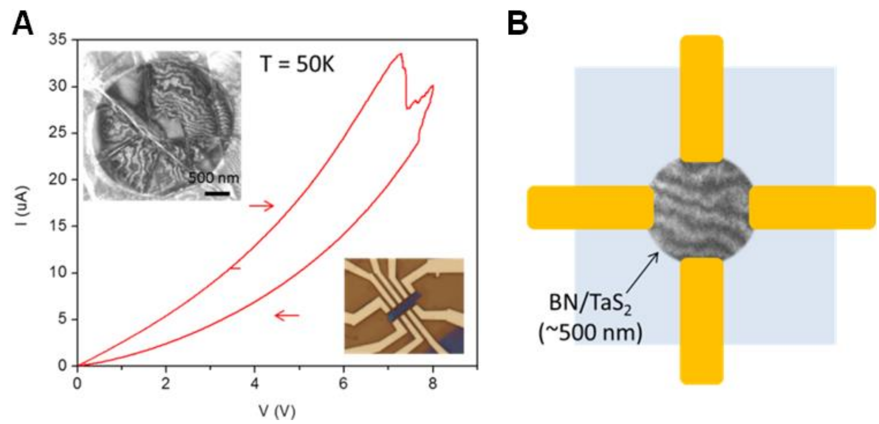

FIGURE 13

Electric transport phenomena in mesocopic charge density wave (CDW) systems. (**A**) (Upper inset) Dark field TEM image of 1T-TaS_2 showing CDW discommensuration network. (Main panel) Nonlinear resistivity and current slip at large bias of device shown in lower inset. (**B**) Device geometry of 1T-TaS_2 nanoisland to measure collective CDW transport and image domain motion in cryogenic TEM.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

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Dr. Joe Qiu
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B. Directorate Scientists

Dr. Thomas Doligalski
Director, Engineering Sciences Directorate

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

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 2014* is to provide information on the programs and basic research supported by ARO in FY14, and ARO's long-term vision for transitioning 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 basic-to-applied research transitions facilitated by this Division in FY14.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Life Sciences Division supports research to advance the Army and Nation's knowledge and understanding of the fundamental properties, principles, and processes 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. In addition to advancing worldwide knowledge and understanding of biological processes, the 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. In addition the Division coordinates 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.

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 FY14, 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.

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, and to reduce the effect of PTSD, suicide, 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 interactions and forces operating at the interface between biological molecules and abiological materials, 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 research in fundamental microbiology and the bioengineering of microbial systems that can help advance needs in Soldier protection and performance. This Program Area is divided into two research Thrusts: (i) Microbial Survival under Environmental Stress and (ii) Analysis and Engineering of Microbial Communities. Research in the Microbial Survival under Environmental Stress 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 antibiotics/antimicrobials and toxins including metals and toxic organic molecules; oxidative stress; and the depletion of specific nutrients. Research approaches include fundamental studies of microbial physiology and metabolism, cell biology, 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 dynamics of microbial-host interactions; and systems level, ecological and evolutionary approaches that examine the relationship and molecular communication within bacterial communities. Research in the Analysis and Engineering of Microbial Communities thrust focuses on the engineering of microorganisms toward biotechnological outputs and applications of interest to the Army. Engineered synthetic microbiological approaches are supported for studies in protein engineering, electromicrobiology, the production of biofuels and commodity chemicals and the bioremediation of toxins. Of joint interest with the ARO Biomathematics Program are research efforts that advance our ability to work with complex biological data sets to increase understanding of microbiological systems, ranging from single-cell processes to multi-cellular interactions.

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 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.

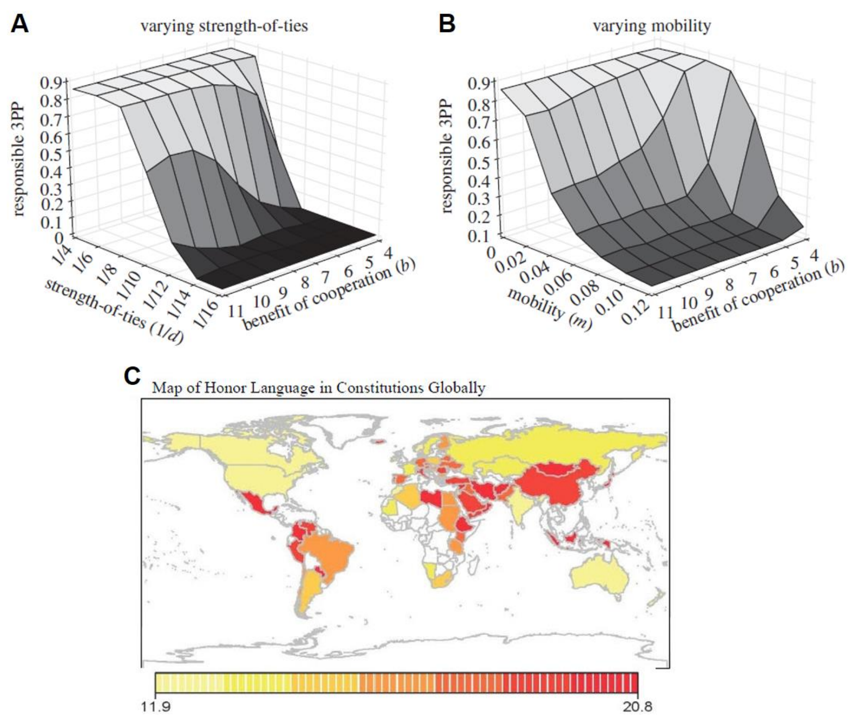

FIGURE 1

Results of research on third-party punishers (3PP) of injustice. This research demonstrated that societies with (**A**) stronger social ties, and (**B**) lower social, there are a higher proportion of actors who will readily disclose deviant activity of community members (i.e., third-party punishers (3PP)). In (**C**), results revealed that this is irrespective of the cultural emphasis placed on honor and allegiance, dispelling the notion that willingness to identify deviant activities and actors in one's community is determined by cultural values and in-group/out-group relations. Instead, it suggests that the analyses of social ties in the community and degree of social mobility act as sensors of information.[1] The color-coding illustrates the degree of cultural emphasis on honor and allegiance; lighter colors (white to yellow) represent countries with lower emphasis; darker colors (orange to red) represent countries with higher emphasis.

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.

[1] Roos P, Gelfand M, Nau D,Carr R. (2014). High strength-of-ties and low mobility enable the evolution of third-party punishment. *Proc. R. Soc. B*. 281:20132661.

C. Research Investment

The total funds managed by the ARO Life Sciences Division for FY14 were $101.8 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY14 ARO Core (BH57) program funding allotment for this Division was $7.3 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 $11.4 million to projects managed by the Division. The Division also managed $60.7 million of Defense Advanced Research Projects Agency (DARPA) programs and $1.9 million for active Minerva Research Initiative projects. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.9 million for contracts. The Institute for Collaborative Biotechnologies received $14.5 million. Finally, $4.1 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.2 million of 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 FY14 (*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 FY14 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 FY14, the Division awarded 18 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to uncover the dynamics of cortical adaptation in auditory perception, to understand new mechanisms of microbial persister cell formation, and to explore conflict and cooperation across social groups. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Susan Aaronson, George Washington University; *State Repression and its Effects on Civil Conflict, Socio-Economic Outcomes, and Leadership Tenure*
- Professor Dana Boatman, Johns Hopkins University; *Multi-scale Dynamics of Cortical Adaptation for Human Auditory Detection*
- Professor Yale Cohen, University of Pennsylvania; *The Spatiotemporal Resolution of Cognitive Signals Revealed Through High-Density uECoG Mapping*
- Professor James Culver, University of Maryland - College Park; *Controlled Microfluidic Assembly and Functionalization of Complex Biomolecules*
- Professor Steven Finkel, University of Southern California; *Long-term Evolution of E. coli: Mutation and Vertical Transmission*
- Professor Sergey Gavrilets, University of Tennessee - Knoxville; *Modeling the Dynamics of Conflict and Cooperation Within and Between Multifarious Social Groups*
- Professor Bart Krekelberg, Rutgers University; *Predicting Brain Electric Currents Through 3D Modeling*
- Professor Jared Lewis, University of Chicago; *Reprogramming Proteins and Enzymes for Transition Metal Catalysis*
- Professor Randolph Lewis, Utah State University; *Spider Silk Glue Proteins*
- Professor Stephen Mitroff, Duke University; *Identifying and Understanding Superior Multiple-Target Visual Search Abilities*
- Professor Alexander Ophir, Cornell University; *Assessment and Screening of Mating Behavior, Behavioral Phenotype and Genotype in African Giant Pouched Rats*
- Professor William Reisinger, University of Iowa - Iowa City; *Why Do Citizens Engage in Bureaucratic Corruption? Political Causes and Consequences of "Illicit Exchanges" in the Post-Soviet Region*

- Professor David Sallach, University of Chicago; *A Mathematical Model of Belief and Influence*
- Professor Gerwin Schalk, Health Research, Inc. - Wadsworth; *Brain-Based Reconstruction of Continuous Silent Speech*
- Professor Peter Scheifele, University of Cincinnati; *Modeling Canine Auditory Cognition and Hearing Acuity Using Electrophysical Techniques*
- Professor Shihab Shamma, University of Maryland - College Park; *Temporal Coherence Principle in Auditory Scene Analysis*
- Professor Stephen Voss, University of Kentucky; *Genetic Management of a Tissue Regeneration Model Organism*
- Professor Thomas Wood, Pennsylvania State University; *c-di-GMP Controls Persister Cell Formation via its Control of Lon Protease Degradation of Antitoxins*

2. Short Term Innovative Research (STIR) Program. In FY14, the Division awarded 11 new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to elucidate the protein structure and subunit functions of forisomes, to examine metabolic and enzymatic activity in dormant Bacillus spores, and to uncover the physiological mechanisms and roles of olfactory sensory integration on visual system function. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Adam Biggs, Duke University; *Assessing and Training Response Inhibition Abilities*
- Professor Edward Dudley, Pennsylvania State University; *Transcriptomics to Identify Alternative Functions of CRISPR-Cas Systems*
- Professor Cheryl Hayashi, University of California - Riverside; *Rapid Characterization of Spider Silk Genes via Exon Capture*
- Professor Michael Knoblauch, Washington State University; *Forisome Based Smart Materials*
- Professor Lei Li, University of Notre Dame; *Improving Visual Perception by Brain Centrifugal Modulation*
- Professor David Melamed, University of South Carolina; *Testing a Mathematical Model of Status Processes and Faction Sizes*
- Professor Peter Setlow, University of Connecticut - Health Center; *Measurement of Metabolic Activity in Dormant Spores of Bacillus Species*
- Professor Zhiyong Yang, Medical College of Georgia Research Institute, Inc.; *A Novel Dataset of Structured Probability Distributions in Natural Scenes*
- Professor Rachel Yehuda, Icahn School of Medicine at Mount Sinai; *Validating Epigenetic Biomarkers for PTSD*
- Professor Lingchong You, Duke University; *Development of a Microfluidic Platform to Analyze Evolution of Programmed Bacterial Death*
- Professor Harold Zakon, University of Texas at Austin; *Analysis of a Novel Microbial Ion Channel*

3. Young Investigator Program (YIP). In FY14, the Division awarded three new YIP projects. These grants are driving fundamental research such as the design of inhibitors that target chromatin to advance the potential for RNA-based mechanisms to control antiviral response. The following PIs and corresponding organizations were recipients of new-start YIP awards.

- Professor Shawn Douglas, University of California - San Francisco; *Programming Biomolecular Nanodevices and Immune Cell Recognition*
- Professor Jinglin Fu, Rutgers, The State University of New Jersey - Camden; *Developing Regulatory Biochemical Reaction Circuits*
- Professor Ivan Marazzi, Icahn School of Medicine at Mount Sinai; *Characterization of Virulence Factor-Mediated Interference with the Human Genome*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY14 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *5th International Workshop on Advances in Electrocorticography*; San Diego, CA; 9-11 November 2013
- *Visual Search: A Comprehensive Treatment*; Washington, DC; 5-6 December 2013
- *11th Conference on the Foundations of Nanoscience*; Snowbird, UT; 14-17 April 2014
- *Biointerface Science Gordon Research Conference*; Il Ciocco, Italy; 14-20 June 2014
- *Neural Interfaces Conference*; Dallas, TX; 21-23 June 2014
- *32nd Federation of American Societies for Experimental Biology Science Research Conference on Virus Structure and Assembly*; Saxtons River, VT; 28 June - 4 July 2014
- *2014 Telluride Neuromorphic Cognition Engineering Workshop*; Telluride, CO; 29 June - 19 July, 2014
- *2014 Human Single Nucleotide Polymorphism and Disease Gordon Research Conference*, Easton, MA; 3-8 August 2014
- *Workshop on Frontiers in Human Brain Mapping: Imaging, Big Data, and Computation*; Princeton, NJ; 26-27 August 2014

5. Special Programs. In FY14, 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 11 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. Exploring Brain-to-muscle Neural Signaling. This MURI began in FY08 and was awarded to a team led by Professor Thomas D'Zmura at the University of California, Irvine. The objective of this research is to investigate brain signals and the corresponding muscle responses. This MURI is co-managed by the Computing Sciences Division and explores similar, but complementary concepts as the Computing Sciences Division MURI led by Professor Gerwin Schalk (see CHAPTER 4: COMPUTING SCIENCES DIVISION).

The team is using electroencephalographic (EEG) readings of the brain, which measure electrical activity along the scalp produced by the firing of brain neurons, to determine whether thought (*i.e.,* unspoken words) can be decoded. The MURI leverages breakthroughs in neuroscience and cognitive science uncovered in recent years. These breakthroughs, when coupled with technological advances in both hardware and software, have significantly advanced research that may ultimately lead to brain-computer interfaces (BCIs) that can decode the activity in brain networks. This potential long-term application is nearly analogous to the development of speech recognition software; however rather than having sound as the input, the inputs will be EEG signals. This concerted research will also attempt to develop a computational model that could decode intended mental speech and decode the direction of the attentional orientation of an individual based solely upon recorded activity from the surface of the scalp.

Preliminary results from the research teams have revealed that the EEG can be used to detect imagined speech rhythm and the pattern of stress in auditory imagery generated by imagined speech. Results from studies of attentional direction have suggested that covert spatial attention engages multimodal parietal areas as well as premotor and frontal areas are activated as part of motor planning for physical orienting (see FIGURE 2). EEG signals generated during lateralized covert attention strongly resemble those used in conventional BCIs to signal left and right through lateralized motor imagery.

Additional results using magnetoencephalography (MEG; a non-invasive technique used to measure magnetic fields generated by the small intracellular electrical currents in neurons) suggest that imagined movements are similar to imagined speech in that an internal forward model generates a somatosensory prediction produced during motor output planning. BCI software under development uses time-, frequency- and time-frequency-domain features of EEG signals to drive navigation and other behaviors in a 3D virtual environment and to drive a tube resonance model for speech synthesis. The evolution of this research beyond the MURI could lead to direct mental control of engineered systems by thought alone, ranging from automobiles to construction equipment to computers.

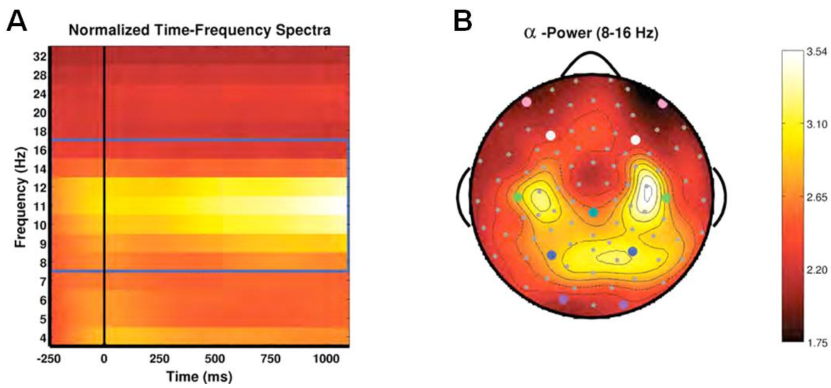

FIGURE 2

Covert spatial attention engages multimodal parietal areas as well as premotor and frontal areas. (**A**) Alpha-band power increases just prior to the 500 msec mark at which stimuli to be attended first appear. Increased power extends through 1,100 msec, the latest time at which stimuli to be attended appear. (**B**) The topographic distribution of alpha power, averaged across time, displays the parietal and fronto-central components characteristic of attentional networks revealed by functional magnetic resonance imaging (fMRI) studies of visual attention.

2. Exploring Signaling Network Interactions Controlling Mouse and Salamander Limb Regeneration. This MURI began in FY09 and was awarded to a team led by Professor Ken Muneoka at Tulane University. The objective of this research is to identify and characterize signaling network interactions that control mouse and salamander limb regeneration.

The ultimate goal of this MURI is to establish the molecular-genetic foundation necessary for limb regeneration. The Mexican salamander is being used as a model organism (see FIGURE 3). The investigators are using a comprehensive approach to document all gene transcripts that are modified during limb regeneration in this model organism. The researchers will use this data to develop a complete regeneration specific microarray chip that can be used to gather data from mathematical modeling of temporal changes in cellular transcriptomes associated with regeneration, in particular, the reprogramming of fibroblasts. The team will model regeneration in the mouse digit tip that is mediated by blastema formation. The modeling is expected to identify specific nodes during the injury response that control whether a wound heals via scar tissue or via reprogramming to form a blastema and eventually regeneration. In the long term, the results of this research could potentially be used to initiate regenerative therapeutics to be tested on amputated limbs in a rodent model.

FIGURE 3

The axolotyl (Mexican salamander). This organism is capable of regenerating most of its body parts, and is being used as a model system for regeneration studies.

3. Mechanisms of Bacterial Spore Germination. This MURI began in FY09 and was awarded to a team led by Professor Peter Setlow at the University of Connecticut Health Science Center. The objective of this research is to decipher the biological mechanisms that underlie heterogeneity of bacterial spore germination with an emphasis on the slow germinating population

Most bacterial spores readily and quickly germinate after being exposed to appropriate growth conditions, a small percentage do not. Within the population, individual spores may germinate days, weeks, or even months, with serious implications. In food processing, the presence of slowly germinating spores results in a need for harsh processing conditions, such as high pressure and temperature, leading to a loss of food quality and appeal. Medically, delayed germination can result in disease appearance after antibiotic therapy has been discontinued. This research team is using a combination of "wet lab" experiments and computational modeling to understand the fundamental mechanisms of spore germination. This research may ultimately lead to strategies for preventing bacterial spore germination that could be used in food processing and medically-relevant therapeutic technologies, and for the enhancement of spore germination to be used in new methods of biofuel production.

4. Modeling Cultural Factors in Collaboration and Negotiation. This MURI began in FY09 and was awarded to a team led by Professor Katia Sycara at Carnegie Melon University. The objective of this MURI is to understand how cultural values, such as the highly-prized "sacred values," can shape the collaboration and negotiation process.

The team has made interesting discoveries in these studies, including the observation of certain values called "sacred values" that are considered as essential to the identity of a given social group, thereby leading members of the group to respond defensively when these values are seen to be challenged or threatened. One example of sacred values includes the observation that the Iranian nuclear program is treated as sacred by some Iranians, leading to a greater disapproval of deals that involve monetary incentives. In addition the team is exploring how humiliation may contribute to regulating relationships within Muslim countries. Humiliation seems to result in clashing behavioral tendencies that offer no regulatory strategies. Participants in the study motivated to change the status quo underestimated the extent to which the out-group moralized the domains of harm, care, fairness and justice. Further, participants motivated to maintain the status quo accurately identified that the out-group moralized harm, care, fairness and justice to the same extent that they themselves did. The investigators will replicate these studies in India and Israel/Palestine in the coming year.

5. 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.

6. 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.

7. 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.

8. 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.

9. 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.

10. 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).

11. 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.[2] 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 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.

12. 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.

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 FY14, the Division managed three new-start SBIR 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 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 FY14, the Division managed five new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects

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[2] 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.

consisted of three Phase I contracts and 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.

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 FY14, the Division managed one new ARO (Core) HBCU/MI project and 19 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 PECASE winners for each calendar year are typically announced by the White House at the end of the fiscal year. However, the 2014 PECASE recipients had not yet been announced at the time this issue of ARO in Review was completed. 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 FY14, the Division managed 11 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. University Affiliated Research Center (UARC): Institute for Collaborative Biotechnologies (ICB)

The ICB 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 ICB 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 ICB 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 $13.6 million was allocated to the ICB in FY14, which was the sixth year of a $120 million contract that was amended in FY14 for the next five-year period. Of these FY14 funds, $11.6 million was allocated for 6.1 basic research and $2.0 million was allocated for four 6.2 projects, including one new project.

In FY14, the ICB supported 66 faculty members, 102 graduate students, and 68 postdoctoral fellows across 15 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 ICB program website (*http://www.icb.ucsb.edu/research*). A U.S. Army Technical Assessment Board and an Executive Steering Board biennially review the ICB research portfolio, assessing the project goals and accomplishments and set goals for the coming year.

I. DARPA Reliable Neural-Interface Technology (RE-NET) Program

The goal of this program is to develop high performance and clinically viable in-vivo neural interfaces to control dexterous functions made possible with advanced prosthetic limbs, enabling service members with amputations to return to active duty and improve their quality of life. ARO Life Sciences co-manages projects in the Reliable Peripheral Interfaces (RPI) focus area, which involves the design, fabrication, testing, and analysis of new materials and technologies to demonstrate substantial improvements in reliability and quantity of peripheral motor-signal information available to drive a neuroprosthetic device. One approach supported through this program involves the translation of surface or intramuscular electromyogram activity to drive neuroprostheses via the recognition of specific electrical activity patterns from residual muscles. This 'intended movement' information enables unprecedented control of robotic limbs. Another approach is exploring the design of a sensory feedback interface from the prosthetic fingers to the user's skin to enable intuitive touch feedback.

J. DARPA Enabling Stress Resistance Program

The goal of this program, co-managed by the Life Sciences Division and DARPA, is to create a comprehensive, quantitative description of the impact of stress on the brain. This research seeks to leverage cutting-edge technologies and recent advances in molecular neurobiology, neuroimaging and molecular pathway modeling as applied to animal models of acute and chronic stress. The objective of this research is a proactive approach to stress mitigation, starting with development of a comprehensive understanding of the complex effects of multiple stressors on the brain. The program has the ultimate goal of the development and implementation of cognitive, behavioral, and/or pharmacological interventions that will prevent the deleterious effects of stress on the brain. The investigators will pursue their objectives through the creation of research teams to thoroughly investigate the multiple physiological pathways and molecular mechanisms involved in the brain's response to acute and chronic stress as well as physical, social, cognitive and affective stressors.

K. DARPA Stochastic Computing Machines Enabled by DNA Self-Assembly Project

The Life Sciences Division currently co-manages a DARPA project focused on creating stochastic computing machines using self-assembled DNA nanostructures. This joint project aims to demonstrate the feasibility of a new class of computing machine that is physically implemented by DNA self-assembly and molecular-scale devices. The computing machine will be based on digital stochastic state machines, unlike traditional digital circuits, which are based around deterministic finite state machines. The planned computing machine has potential to deliver improved performance at vastly reduced power and size by using architectures that are implemented using nanoscale physical devices.

L. 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.

N. Department of Defense Forensic and Biometric Research and Development Program

The goal of this program, co-managed by the Life Sciences Division and DFBA, is to enhance the capability of forensic science and biometric applications for DoD customers both in traditional law enforcement/criminal justice purviews and in expeditionary environments. Two projects initiated in late 2012 continued in this third year of the program. The first is focused on statistical analysis of firearms and aims to develop a system to allow for examiner-independent evaluation of impressions generated by the discharge of a firearm using Integrated Ballistics Identification System (IBIS) data. In the expeditionary environment, the proposed system will provide a useful measure of match statistics, reducing time and potentially the need for a verification step, allowing a single examiner to make decisions on firearm comparisons. The second project aims to identify body fluid-specific gene transcripts and incorporate them into an RNA-based body fluid multiplex identification system. The proposed system will enhance forensic capabilities of DFBA 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. In addition, a third project was awarded in 2014 which will evaluate 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.

O. DARPA Rapid Threat Assessment (RTA) Program

The goal of this program is to develop methods and technologies that can, within 30 days of exposure to a human cell, map the complete molecular mechanism through which a threat agent alters cellular processes. The program is co-managed by the Life Sciences Division, which involves participation and leadership in proposal evaluations, selections, monitoring, and site visits. Research challenges include developing tools and methods to detect and identify the cellular components and mechanistic events that take place over a range of times, from the milliseconds immediately following threat agent exposure, to the days over which alterations in gene and protein expression might occur. Understanding the molecular mechanism of a given threat agent would provide researchers the framework with which to develop medical countermeasures and mitigate threats. If RTA is successful, potential adversaries will have to reassess the cost-benefit analysis of using chemical or biological weapons against U.S. forces that have credible medical defenses.

P. 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 and FY13. Project selection and funding began in FY09. There were five active projects pursuing research under this topic in FY14.

Q. Minerva Research Initiative (MRI) Topic: Science, Technology, Political, and Military Transformation in China & Developing States

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), 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 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, and political governance 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, and FY13. Project selection and funding began in FY12. There were four active projects pursuing research under this topic in FY14.

R. 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, and FY13. Project funding and selection began in FY12. There were seven active projects pursuing research under this topic in FY14.

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. Organic Matrix Templating and Function in an Ultrahard Biological Composite

Professor David Kisailus, University of California – Riverside, Single Investigator Award

Efficient strategies have evolved to synthesize materials that often exhibit exceptional mechanical properties, exemplified in the mineralized tissues of numerous species. These biological systems demonstrate the ability to control nano- and micro-structural features using organic templates that not only precisely guide the formation and phase development of minerals, but also significantly improve the mechanical performance of otherwise brittle materials. One such example is found in the heavily mineralized radular teeth of the chitons, a group of elongated mollusks that graze on hard substrates for algae. The radula, toothed ribbon-like structures which are used for this feeding are well known for their ability to efficiently erode the rocky surfaces on which the chitons feed (see FIGURE 4). Professor David Kisailus at the University of California - Riverside is exploring synthesis-structure-property relationships in unique biomaterials that exhibit remarkable damage tolerance and abrasion resistance.

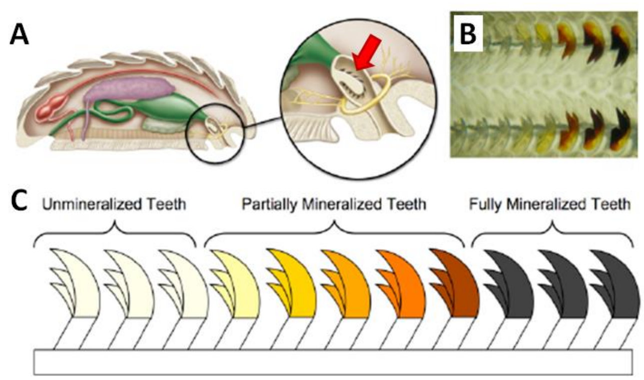

FIGURE 4

The damage tolerant and abrasion resistant radular teeth of chitons. Professor Kisailus will explore the chemical and structural features of the mineralized radular teeth of chitons to elucidate structure-property relationships in these unique damage tolerant and abrasion resistant biological composite materials. (**A**) The internal anatomy of a chiton identifying the location of the radula (red arrow), a toothed conveyor belt-like structure used for feeding. (**B**) A photographic image of the mineralized teeth of the radula. New teeth are continually formed and are mineralized as they migrate toward the functional feeding position. Thus this system provides Professor Kisailus with unmineralized teeth, partially mineralized teeth and fully mineralized teeth for analysis (**C**).

The overall goal of this project is to investigate the chemical and structural features of both the fully mineralized radular teeth of the chiton Cryptochiton stelleri and the underlying organic framework which provides a template for mineral growth and a scaffold for the teeth. In FY14, proteins that compose the underlying organic framework of the radular teeth were isolated and identified by protein sequencing. Several proteins were dominant in the fully mineralized part of the teeth, including myoglobin and a highly acidic peptide. Myoglobin may play an important role the mineralization process by controlling the oxygen level to promote iron oxide mineralization. The highly acidic peptide could be involved in iron oxide precipitation within the cusp of the tooth, however further analysis of the entire protein sequence will be needed to fully elucidate its function in the mineralization process.

In addition, in FY14 the phase transformations and structural developments that occur during mineralization were characterized using a variety of imaging techniques, including x-ray diffraction, micro-x-ray fluorescence and electron microscopy. The results revealed a process initiated by the deposition of ferrihydrite aggregates at the leading edge of the tooth tips, followed by phase transformation of the aggregates to solid-state magnetite, followed by magnetite crystal growth to form rods (see FIGURE 5). Notably, this analysis indicated that the underlying protein matrix appears to influence the density of the aggregates and the diameter and curvature of the fully formed magnetite rods, both of which are likely to play critical roles in determining the mechanical properties of the fully mineralized teeth.

Professor Kisailus will build upon these results to design a biomimetic in vitro mineralization process to understand the organic-inorganic interactions and mineral growth mechanisms that lead to the architectural features of the radula that enhance abrasion resistance and damage tolerance. This project will provide fundamental understanding of synthesis-structure-property relationships in unique abrasion resistant and damage tolerant biological composite materials that may enable the future development of the necessary tools for the design and fabrication of cost-effective and environmentally friendly engineered materials that mimic key design elements and performance properties present in biological systems.

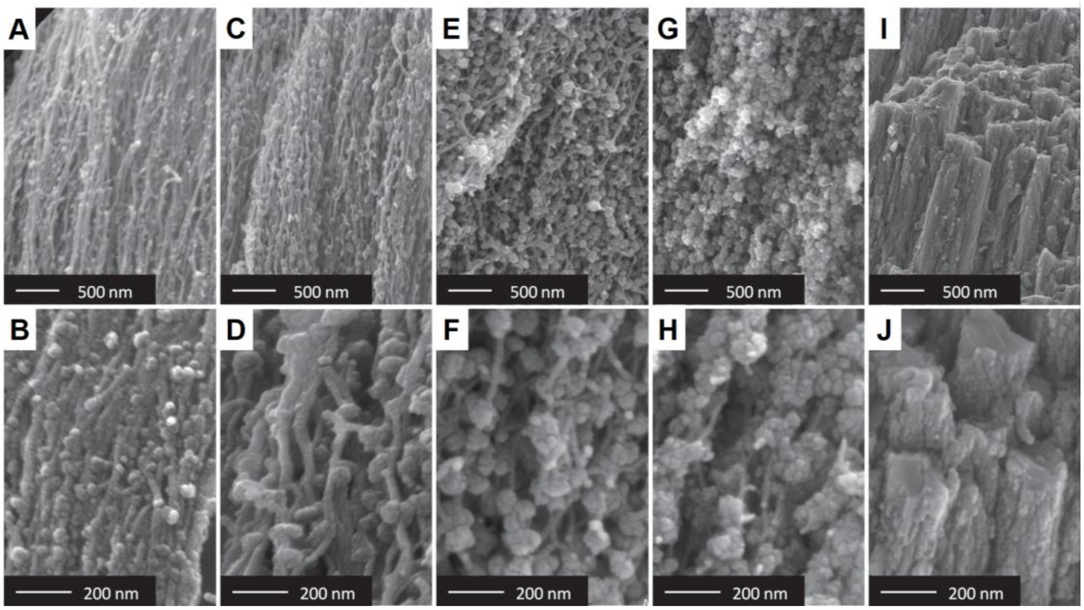

FIGURE 5

Sequential stages of magnetite rod formation during radular tooth mineralization. Scanning electron microscopy analyses of fracture surfaces from the tips of developing radular teeth. The mineralization process begins with deposition of ferrihydrite aggregates [(**A**,**B**) Tooth #1]. The aggregates then begin phase transformation to solid-state magnetite [(**C**,**D**) Tooth #2], and continue to grow [(**E**,**F**) Tooth #3, (**G**,**H**) Tooth #4], ultimately forming continuous rods in fully mineralized teeth [(**I**,**J**)].

B. Communication Between the Endoplasmic Reticulum and Mitochondria

Professor Eric Schon, Columbia University, Single Investigator Award

Mitochondrial interactions have been implicated in certain neurodegenerative diseases (see FIGURE 6). The objective of this research is to analyze mitochondria-associated endoplasmic reticulum membrane function in human induced pluripotent stem cells differentiated into neurons and tissues from presenilin-1 knock-in mice, to investigate how endoplasmic reticulum-mitochondrial tethering affects mitochondria-associated endoplasmic reticulum membrane function, and to conduct proteomic analyses of normal vs presenilin mutated mitochondria-associated endoplasmic reticulum membranes in order to identify and understand the factors associated with endoplasmic reticulum-mitochondrial communication.

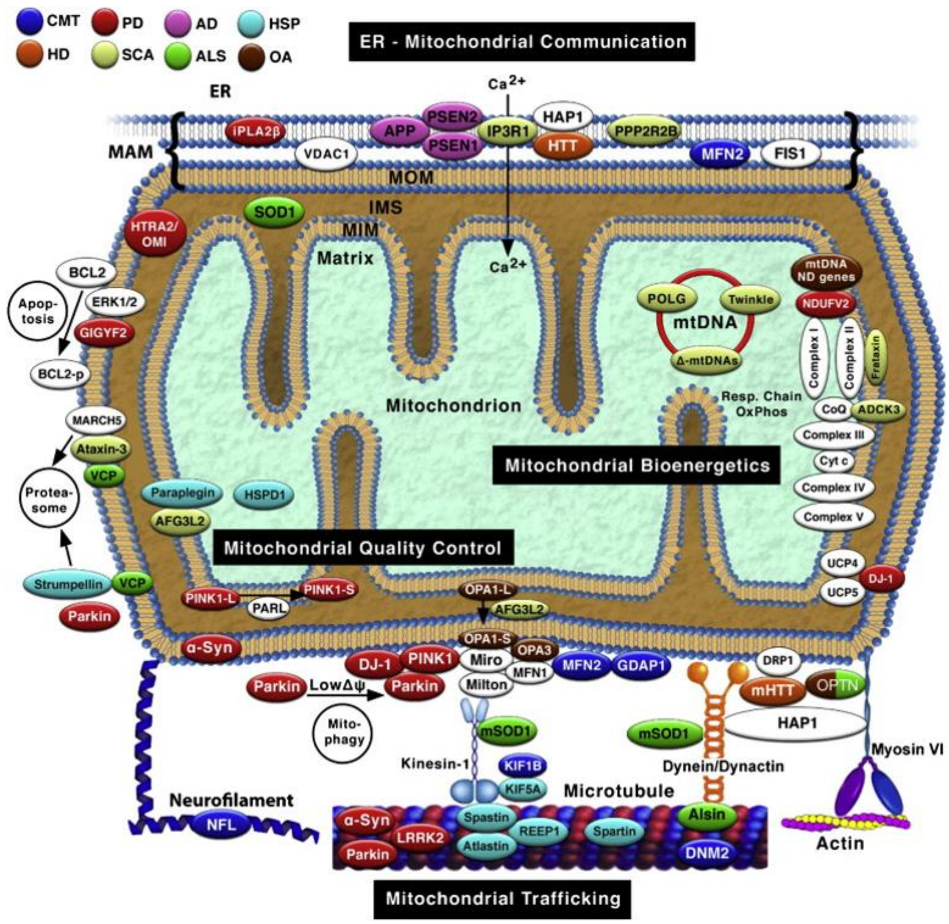

FIGURE 6

Mitochondrial interactions in neurodegenerative diseases. Proteins associated with mutations causing neurodegenerative disorders are in colored ovals and are associated with four broad mitochondrial functions. Proteins that "touch" each other indicate an established physical or genetic interaction. For simplicity this figure does not show all interactions.[3]

The investigators discovered that, contrary to the dominant view in the field, presenilin-1 and presenilin-2, catalytic components of the gamma-secretase complex, are not present homogenously in the endoplasmic reticulum, but rather are present heterogeneously. Specifically they are highly enriched in the mitochondrial-associated endoplasmic reticulum membranes. They discovered that the lower activity uncleaved form of presenilin-1 is present throughout the endoplasmic reticulum, and that the active processed form of the protein is present almost exclusively in the mitochondrial-associated endoplasmic reticulum membrane. Secondly, they discovered that persons with either familiar or sporadic Alzheimer disease have massively increased endoplasmic reticulum-mitochondrial connectivity and mitochondrial-associated endoplasmic reticulum membrane activity, which sheds light on the phenotypic consequences of the disease. Thirdly, they discovered that ApoE4 (the largest known genetic risk factor for late-onset sporadic Alzheimer disease) upregulates mitochondrial-associated endoplasmic reticulum membrane function relative to ApoE3, which provides a mechanistic explanation of the elevated risk factor in humans with ApoE4, and also points to the significance of upregulated mitochondrial-associated endoplasmic reticulum membrane function as a unifying principle underlying both familial and sporadic Alzheimer disease. Fourthly, they determined that increase endoplasmic reticulum-mitochondrial connectivity via mitochondrial-associated endoplasmic reticulum membranes is almost certainly the cause of the established decrease in mitochondrial respiratory chain and oxidative phosphorylation activity in patients with Alzheimer disease, which often precedes the onset of plaque formation by years, establishing that reduced

[3] Schon EA, Przedborski1 S (2011). Mitochondria: The Next (Neurode)Generation. *Neuron*. 70:1033-1053.

oxidative phosphorylation is not a downstream side effect but rather a direct consequence of upregulated mitochondrial-associated endoplasmic reticulum membrane function. This discovery also points out a heretofore unknown mechanism by which a cell can modulate its bioenergetic output in real time in response to cellular bioenergetic needs.

In summary, these results identify Alzheimer disease as fundamentally an aberrant endoplasmic reticulum-mitochondrial connectivity disorder, with the plaques and tangles being a downstream side effect rather than a causal feature. In the short term these results offer new directions for prevention, diagnosis, and treatment of Alzheimer disease. In the long term this new fundamental understanding of mitochondrial energetic capabilities, mitochondrial-endoplasmic reticulum communication, and mechanisms of cognitive decline will enable future investigators to develop new approaches to preventing cognitive decline in aging and injured warfighters, and to develop new therapeutic approaches to maintain and enhance warfighter cognitive performance capabilities.

C. Enhancing Sensory Perception with Ultrasound

Drs. Sumon Pal and William Tyler, Thync, Inc., SBIR Contract

The objective of this research is to modulate the human perceptual bandwidth and cognitive function using low intensity, low frequency, pulsed ultrasound to safely and reliably modify neuronal excitability. Possessing the ability to noninvasively and remotely elicit brain circuit activity yields immense experimental and therapeutic power. Ultrasound as a means of exciting and reversibly suppressing neuronal activity was shown to be effective on a gross level several decades ago. Since then, explorations into the use of ultrasound as a neurostimulation tool have been relatively sparse. The focus has instead been on employing more traditional approaches such as pharmacological, electrical, magnetic, and photonic stimulation of neuronal circuits. The coupled ability of ultrasound to directly stimulate neuronal activity and to provide noninvasive transmission through bone and other biological tissues in a focused manner holds promise as a potentially powerful neuromodulation tool.

In FY14, researchers at Thync, Inc. and Virginia Tech demonstrated the first use of ultrasound to enhance sensory perception by modulating human brain activity. This groundbreaking finding, published in *Nature Neuroscience*, revealed that low-intensity ultrasound could be delivered from a noninvasive device to enhance tactile awareness (see FIGURE 7).[4] This new method was made possible by prior ARL-ARO funded basic research using animal models at Arizona State University, where investigators discovered how particular brain regions can be stimulated using ultrasound to control specific muscles. These results mark the beginning of an emerging research area. Researchers are considering follow-on research to develop noninvasive tools to modulate performance under physical stress, fatigue, or cognitive overload and to modulate the human informational bandwidth capability.

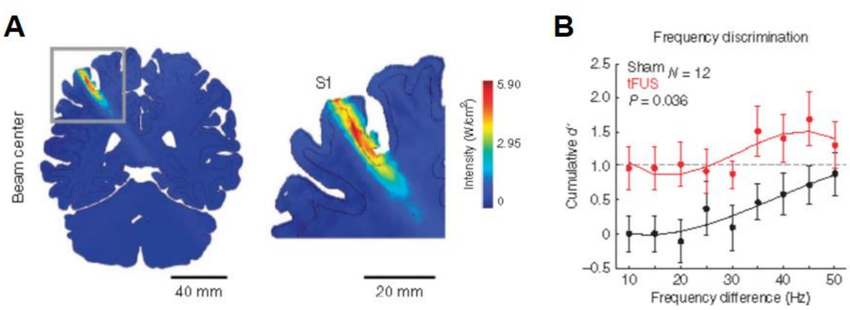

FIGURE 7

Transcranial ultrasound neuromodulation. Transcranial focused ultrasound (fFUS) can be targeted to spatially discrete regions of human cortex and enhances sensory discrimination abilities. (**A**) Coronal cutaway view showing the acoustic intensity field of the focused ultrasound beam projected into a realistic finite element model of the brain derived from whole-head structural magnetic resonance images. (**B**) Psychophysical data from sham or tFUS treatment during frequency discrimination tasks. tFUS significantly lowered sensory discrimination thresholds (d' closer to 1).[4]

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[4] Legon W, Sato TF, Opitz A, Mueller J, Barbour A, Williams A, Tyler WJ. (2014). Transcranial focused ultrasound modulates the activity of primary somatosensory cortex in humans. *Nat Neurosci*. 17:322-329.

D. Quantitative Monitoring of Bacterial Quorum Sensing Behaviors

Professor Marvin Whiteley, University of Texas at Austin, Single Investigator Award

Bacteria can display social behavior in the form of quorum sensing which allows microbial cells to communicate with each other through excreted extracellular chemical signals. Once a critical cell mass accumulates within a bacterial colony, a signaling threshold is reached that can trigger expression of specific sets of genes within the microbes in a colony and with neighboring colonies thereby affecting community behavior. In the pathogenic bacteria *Pseudomonas aeruginosa*, a microbe frequently found in infected wounds, a quorum sensing response can activate the expression of genes that encode various toxins and proteases that can contribute to virulence within a wound. The goal of this research is to determine the cell density and colony patterning required to activate the quorum sensing-mediated expression of these virulence factors. The PI has developed a system that controls colony aggregate size and spatial arrangement *in vitro* via micro-3D printing of gelatin-based microtraps that surround nascent microbial colonies. The crosslinking of the gelatin within the walls and ceiling of these traps is tuned to enable diffusion of signaling molecules while retaining the bacteria within the trap. Professor Whiteley's laboratory demonstrated that individual traps can be designed to any size or shape and the distance between neighboring colonies can be tuned and controlled (see FIGURE 8).

Professor Whiteley's laboratory has coupled this platform with an electrochemical assay for detection of pyocyanin (PYO), a redox-active virulence factor produced and secreted by *P. aeruginosa* as part of the quorum sensing response, and scanning electrochemical microscopy (SECM) to detect the presence of PYO above the permeable roof of a microtrap. As a colony develops within a trap, 3D confocal microscopy provides a means of quantify cell count and the SECM current measurements provide an indicator of a quorum sensing response in the presence of PYO. His initial experiments have utilized two *P. aeruginosa* variants confined within neighboring traps: one variant can produce a quorum sensing signal while the other can produce the PYO responder. These experiments have shown that aggregates larger than 2,000 bacteria are required to trigger this form of quorum sensing behavior when neighboring aggregates are positioned 8 microns from each other. By systematically varying the size and distance of neighboring traps, one can determine the full range of conditions required to affect quorum sensing. Whiteley's group is planning additional experiments with this platform to define the determinants that trigger quorum sensing in the presence of a two different pathogenic species. For example, it has been shown that laboratory co-cultures of *P. aeruginosa* and *Staphylococcus aureus*, another common pathogen found in infected wounds, exhibit an enhanced induction of *P. aeruginosa* virulence factors. This platform will then be systematically engineered to study and quantify the interactions between these two pathogens in a controlled spatial environment.

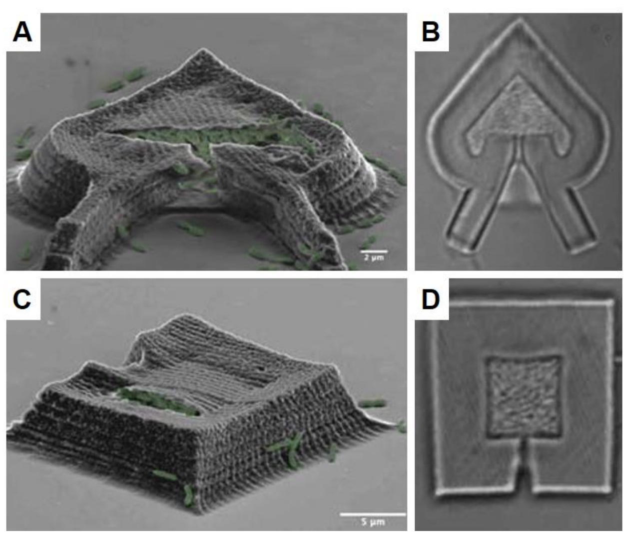

FIGURE 8

Bacterial microtraps containing *P. aeruginosa*. For these experiments, a single bacterium was trapped and monitored throughout growth. Scanning electron micrographs of (A) 2 pL heart-shaped and (C) 2 pL square traps are shown with the roof torn to expose the bacteria (false-colored green). Phase contrast micrographs of (B) heart-shaped and (D) square traps filled with *P. aeruginosa*. The capacity of these traps is approximately 2000 *P. aeruginosa*. Scale bar in A is 2 μm and in C in 5 μm.

E. Assessing Trustworthiness in Social Media: A Social Computing Approach
Professor Huan Liu, Arizona State University, Single Investigator Award

Social media are a rich source of information about individuals and their affiliations, intentions, opinions, and social influence vis-à-vis others with whom they interact. How that information and the sources of it are interpreted and used (often maliciously), and identifying the sources and levels of risk for individuals (e.g., identity theft, identity destruction) are not well understood. The challenges are compounded by the volume of data and the computational challenges that presents for efficient and accurate analyses of social media to detect groups and communities, identify influential actors in those communities, and detect vulnerabilities to malevolent use of information available through social media. Importantly the underlying social mechanisms theorized by social scientists to underlie these dynamics have been difficult to represent in existing research models. A goal of Professor Huan Liu at Arizona State University is to demonstrate how social theories, such as homophily, balance theory, and status-influence theory capture fundamental structural dynamics that can improve algorithm development in the analysis of textual media.

Professor Liu's research has demonstrated methods through which social theories can systematically inform algorithm development to mine social data for particular types of information. He notes that a challenge for data mining is that social media data tend to be big, noisy, incomplete, and unstructured. Yet, strategically applying social science theory to guide the data mining algorithms can overcome this challenge, because many social science theories are designed to predict the structure of a social system from incomplete information. Consequently, Professor Liu's research is developing more effective and efficient data mining algorithms based on social theory to address a range of issues, including detecting privacy vulnerabilities; discovering dark networks; identifying cliques that are more likely to form coalitions, remain neutral towards one another, or become adversarial; detecting the credibility of different actors in a community of social network users; modeling how opinions form and diffuse over across social media users to distinguish the majority from minority perspective (see FIGURE 9).[5]

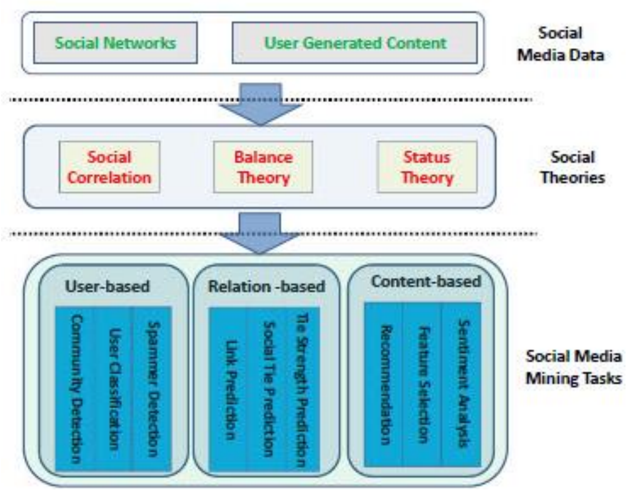

FIGURE 9

Integrating social science theory to facilitate algorithm development. Conceptual representation of strategy for integrating exemplary social theories in algorithm development to mine social media to bridge the gap between the data, its social meaning, and the implications of those meanings.

Professor Liu's research has shown that content becomes linked through the users. Features of the content can also be used to predict the nature of relations among the users, through social theories. Overturning one of the most foundational assumptions of traditional data mining and machine learning methods, the PI's approach demonstrates that, in fact, social media data are not independent, nor are they identically distributed. Importantly, by incorporating social science theory in the development of algorithms to mine social media, this research is forging new ways to detect missing links and content when information is absent (see FIGURE 10).

[5] Tang J, Chang Y, Liu H. (2013). Mining Social Media with Social Theories: A Survey. *ACM SIGKDD Explorations*. 15:20-29.

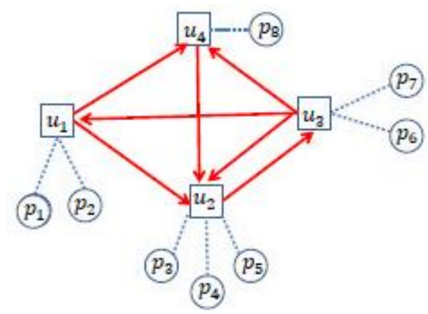

FIGURE 10

Detecting social relations and content from social science theory and data mining methodologies. Examples of social relations and content that can be detected in social media when information is incomplete, where u_i represents social media users, and p_i represents content they may produce.

This exciting research opened new avenues for addressing the challenges of extracting information from social media data, consisting of millions of micro-exchanges between users. It also offers a promising new computational strategy for developing and validating social theories and determining the scalability of dynamics from small groups to interconnected communities of millions of members.

F. Modeling Cultural Factors in Collaboration and Negotiation

Professor Katia Sycara, Carnegie Mellon University, MURI Award

The overall goal of this project is to develop validated cross-cultural theories of collaboration and negotiation that account for cognitive and socialization processes as they relate to the sacred values of actors embedded in complex social networks. The project involves a multi-method approach, which includes experiments, survey research, and field ethnographies to document how negotiations play out under conflict scenarios. One critical thrust of this research is developing models to predict outcomes of conflict negotiations, taking into account the unique values of negotiators from different cultures. Theoretically representing how cultural values affect negotiation strategies and outcomes has been challenging, because values vary widely across individuals from different cultures, creating difficulties for a generalizable theoretical strategy. Consequently, most conventional models of negotiation represents outcomes as a function of optimizing material gains, while avoiding collapse of negotiations, and assigning deviance from these models and observed outcomes to an error term (often attributed to individual value differences). These error terms were often unacceptably large in prior research.

In FY14, members of the Sycara research team published a paper demonstrating a highly successful new method of modeling negotiation outcomes using Inverse Reinforcement Learning (IRL).[6] The premise behind this strategy is that patterns of behavior corresponding to values and hence, likely outcomes, can be learned during the course of negotiation. Through a series of experiments, the researchers established that the IRL model offered a superior fit to observed data and that negotiations do, in fact, depend heavily on complex trade-offs between multiple goals, which reflect distinct cultural values (see FIGURE 11). Professor Sycara's team is the first to integrate the IRL method with game-theoretic strategies to model outcomes in an ultimatum game, which reflects empirical instances of negotiation. It allows for the incorporation of complex and differing values across negotiators, which better represents the real-world dynamics and likely outcomes of cross-cultural conflict resolution.

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[6] Nouri E, Grogila K, and Traum D. (2014). Culture-specific models of negotiation for virtual characters: multi-attribute decision-making based on culture-specific values. *AI and Society*. DOI 0.1007/s00146-014-0570-7.

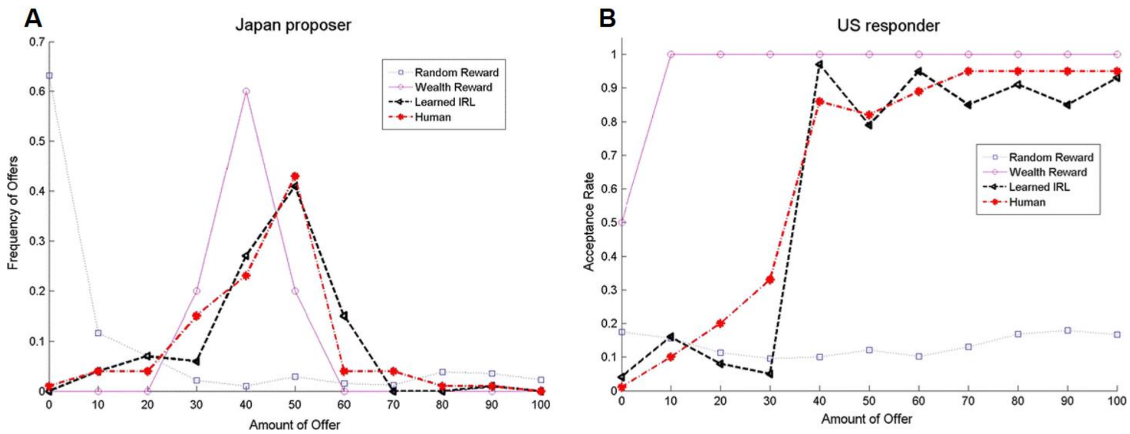

FIGURE 11

IRL model performance. The data plots illustrate the performance of IRL model to observed human behavior and traditional models based on random reward and utility maximization. (**A**) Superior fit of the IRL model for offers (i.e., proposers) in a negotiation, compared to a random reward model and a wealth reward model that corresponds to utility maximization. (**B**) Fit of the IRL model to responders to an offer made by a proposer. In both cases, as shown by the convergence of the red and black lines, the IRL model demonstrates a vastly superior fit, compared to random and utility maximization models.

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 to external organizations and customers.

A. Enhancing Visual Attention through the Sense of Touch

Investigator: Dr. Gary Zets, SBIR Award
Recipient: Engineering Acoustic Inc.

Spatial disorientation is attributed as a leading cause of aviation mishaps in Operations Enduring Freedom and Iraqi Freedom. Helicopter and vertical take-off and landing programs across all services have identified degraded visual environments as the leading cause of spatial disorientation and an urgent problem. Modern aircraft utilize state of the art avionics systems that provide improved visual cueing to aircrew. However, despite significant improvements in cockpit visual displays, there has been no significant reduction in spatial disorientation accident rates. The objective of this project is to develop a system that would accept data from various aircraft sensors and present this information to a pilot or aircrew via tactile, or touch, cueing in an effort to reduce the burden on cognitive resources devoted to vision. The sense of touch offers a relatively untapped and intuitive sensory channel for both communication and orientation. Engineering Acoustic Inc. developed vibrotactile stimulators or "tactors", strategically placed them in the seat cushions of a flight simulator and developed a tactile language to enable research on tactile cueing as a method to reduce cognitive load during simulated flight.

The U.S. Army Safety Center determined that this technology developed through this project, had it been available for the past 20 years, could have prevented 24% of all Army Class A helicopter accidents. In FY14, Engineering Acoustic's tactors, tactile arrays and the associated hardware and software systems transitioned to the U.S. Army Aeromedical Research Laboratory. The effort in FY14 provided the necessary hardware and software upgrades to create new shoulder tactor arrays that were incorporated into seat electronics to provide high altitude information. This relatively small change in the addition of shoulder tactors will permit significantly increased capabilities for the pilot and will aid immensely in the transition of this technology into the cockpit for demonstration to potential military and civilian aviation users. The transitioned system provides a dedicated, standardized, aircraft independent, quickly deployable hardware/software solution that will provide the basis for future research and commercial viability that can also benefit land vehicle and dismounted missions in addition to civilian aviation needs.

B. Prokaryotic Genomic Instability

Investigator: Profs. P. Foster, M. Lynch, H. Tang, Indiana University and Prof. S. Finkel, USC, MURI Award
Recipient: Defense Forensic Science Center

The objective of this research is to provide the first-ever characterization of the fundamental parameters of the prokaryotic mutation process, including both cell-mechanistic and evolutionary components. The research 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 will then extend 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 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 will be analyzed in the context of the mutational signatures of individual repair pathways throughout the genome.

The investigators have discovered that the mutation rate of Escherichia coli, the most researched organisms in the world, is only a third of that predicted by all previously published data. This is due to the fact that all previous mutation rate analyses relied on reporter genes; this first ever analysis of mutation rates and patterns at a genomic level indicated that relying on reporter gene constructs has some fundamental, previously unknown, weaknesses. They also determined that deficiencies in error-prone polymerases, alkylation repair, or nucleotide excision repair had little effect on mutation rates or spectra. Deficiencies in base excision repair did increase the mutation rate and change the base-pair substitution mutational spectra. The most dramatic result was seen with a 7,8-dihydro-8-oxoguanine knockout which increased the mutation rate one hundred fold. Together these results indicate that oxidative DNA damage is the primary cause of mutations in prokaryotic cells growing in culture.

This genomic analyses of mutation patterns also revealed, for the first time, that the density of base-pair substitutions falls into a symmetrical wave-like pattern that is nearly identical in the oppositely-replicated halves of the genome (replicores). The peaks of these waves are in highly transcribed regions of the genome, suggesting that transcription is interfering with DNA replication. The investigators also initiated a global analysis of transcription error frequency and determined that 0.1% of transcripts in Escherichia coli and Saccharomyces cerevisiae contain at least one erroneous base. This suggests that transcription errors are likely to have a significant impact on organismal fitness.

The investigators also developed a new computational framework that is capable of characterizing insertions, deletions, and recombination events of mobile genetic elements based on the A-Bruijn data structure. They continue to work to develop a clustering algorithm to derive valid clusters of discordant read pairs, each supporting a different structural variant event. The structural variant detection framework was applied to a large number of mutation accumulation lines derived from 28 Escherichia coli strains, resulting in the identification of 1296 insertion or recombination events, and indicating that the rate of recombination is constant regardless of the base-pair mutation rate. This results also showed that the birth and death rates of insertion sequence elements is about 3.7×10^{-4} and 1.4×10^{-5} per genome per generation, respectively, when no selection pressure is present (see FIGURE 12).

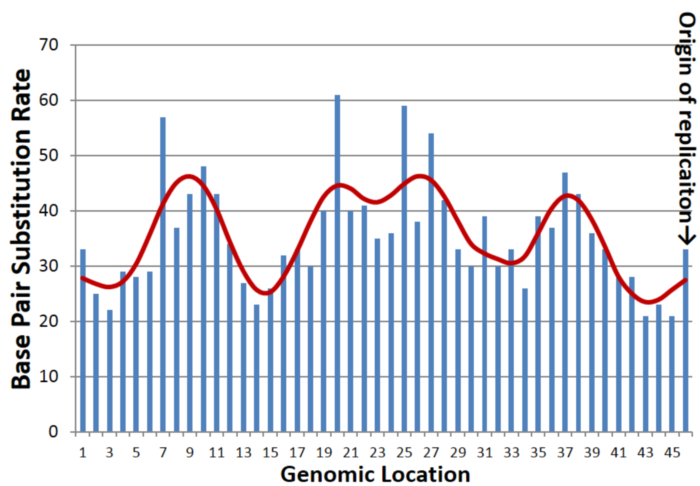

FIGURE 12

Mutational density is distributed in a wave-like pattern across the *E. coli* chromosome.

Correlations between measurements of the base-substitution mutation rate per effective genome size and effective population size, with effective genome size representing the amount of functional DNA in a genome, approximated by the size of the proteome, had been previously reported. The scaling of mutation-rate evolution to the amount of functional DNA in a genome is in accordance with the hypothesis that selection operates to reduce the genome-wide deleterious mutational burden, with the absolute lower limit determined by the power of random genetic drift. This hypothesis, coined the "drift-barrier hypothesis," provides a universal explanation for the evolution of the mutation rate across cellular life. However, there was a potential circularity in the first analyses, because estimates of effective population sizes require estimates of base-substitution mutation rates, so a more independent analysis was desirable. To accomplish this task, the investigators estimated the rate of insertion-deletion mutation events from their cumulative set of mutation-accumulation experiments, which provided a measurement of mutation-rate variation that is independent of that of effective population size. This resulted in the discovery of a near-exact inverse relationship between the rate of insertion-deletion mutation events per effective genome per generation and effective population size across cellular life. This result supports the hypothesis that the ultimate level of refinement for the traits involved in determining the mutation rate of an organism is determined by the drift barrier. The near-exact scaling between the refinement of base-substitution mutation rates and the refinement of the rate of insertion-deletion mutation events reflects the consistency of the drift barrier in governing mutation-rate evolution. Importantly, the drift-barrier hypothesis is a general hypothesis that applies to all biological traits, implying that the maximum refinement of many other molecular and cellular traits may also be inversely related to species-specific levels of random genetic drift.

These investigators were invited to the Defense Forensic Science Center to present their results, where the results transitioned for future study to determine the provenance of items containing prokaryotic DNA.

C. Stable, High Affinity and High Selectivity Protein Capture Agents for Improving Bio-Detection Assays
Investigator: Professor James Heath, ICB - Caltech (UARC)
Recipient: Edgewood Chemical Biological Center (ECBC)

The goal of this research is to explore new approaches for designing protein capture agents that exhibit affinity and selectivity characteristics similar to the gold standard of monoclonal antibodies. The research team has developed three protein capture agents (PCC) against targets within the critical reagents repository, and the lndi Molecular team has worked with the ARL researchers to translate the PCC Agent technology into their laboratory. The developed PCC Agents include anthrax protective antigen (PA). This work was published in a joint publication, and the reagents have undergone rigorous testing at Edgewood to demonstrate a remarkable level of thermal, chemical, and biochemical stability. A state-of-the-art dual capture agent/inhibitor against botulinum neurotoxin serotype A with a dissociation constant of ~100 picoM and the ability to both protect and rescue neuronal cells from BoNT intoxication has been developed. The three scientific advances developed in Heath Lab that were used in the BoNT work are (i) the use of macrocyclic peptide libraries as the basis for PCC agent development, (ii) the use of MALDI TOF/TOF as a sequencing tool for analyzing screening results that utilize the macrocycle peptide libraries, which are already the subject of an issued patent, and (iii) the exploitation of the tertiary structure of the protein target for developing a PCC agent that exhibits true cooperative binding, which is largely what enabled the BoNT studies and what enabled the team to develop a PCC agent with a low picoM binding (and inhibitory) affinity. These discoveries have transitioned to ECBC for the study of the stability characteristics of PCC agents.

D. Deep Ultraviolet Microscopy for the Detection, Quantification and Characterization of Microbes
Investigator: Professor Kenneth Nealson, University of Southern California, Single Investigator Award
Recipient: NASA

The objective of this research is to utilize deep ultraviolet (DUV) microscopy for the detection, quantification and characterization of microbial life on a variety of different opaque surfaces. DUV takes advantage of the natural fluorescence of aromatic amino acids found in proteins. The main objective of the effort is to bring together a DUV microscope and Raman system where the DUV microscope is used to identify the presence of microbes in real time and the Raman system is used to gain detailed chemical information that could be used to identify the microbes and specific aspects of their metabolism. Using these methods, Nealson' group has successfully been able to quantify microbes on surfaces of filters, develop reproducible Raman signatures for four different bacterial species, and optically distinguish between vegetative cells and spores.

Given the ability to provide luminescent detection of organics and the versatility of this technology to probe for organics on a variety of different surfaces, the DUV microscope transitioned to the NASA Jet Propulsion Laboratory to include as an effective instrument for NASA missions, particularly the Scanning Habitable Environments with Raman & Luminescence for Organics and Chemicals (SHERLOC) system for use in the Mars 2020 Rover Mission. The combined use of DUV and Raman will then provide SHERLOC with the ability to probe for the presence of specific organics on the Martian surface which could provide clues to whether past life has been preserved.

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. Spider Silk Glue Proteins

Professor Randy Lewis, Utah State University, Single Investigator Award

Orb-web weaving spiders produce a web containing, as its major element, a spiral responsible for both stopping flying prey and preventing their escape. This spiral is composed of two key elements, a pair of flagelliform silk fibers which have a very high elasticity, and an adhesive glue secreted from the aggregate glands. The aggregate gland glue is initially uniformly layered on the flagelliform fibers, but spontaneously forms a series of evenly spaced droplets (see FIGURE 13). While preliminary studies have suggested that the aggregate gland glue is the strongest biological adhesive ever tested, it is extremely challenging to separate the glue from the silk it covers for testing. To circumvent this research challenge, the goal of this project is to recreate the glue separately to determine the true properties of this biological adhesive on a macro-scale. The glue will be recreated by expressing the two proteins that form the glue in an insect cell culture system.

While the genes that encode the glue proteins have been identified, the complete gene sequences have not yet been assembled. It is anticipated that in FY15, the full-length genes encoding the two glue proteins will be generated and incorporated into the insect cell culture system for recombinant production. This will provide a foundation for production of sufficient quantities of the proteins to enable testing of the adhesive properties of each protein individually, as well as in various ratios.

Professor Lewis' research will provide fundamental understanding of a biological adhesive that appears to have extraordinary strength and is highly tolerant of a wide variety of environmental conditions. This research may enable the future development of synthetic adhesives that provide advanced capabilities for military and commercial applications irrespective of environmental operating conditions.

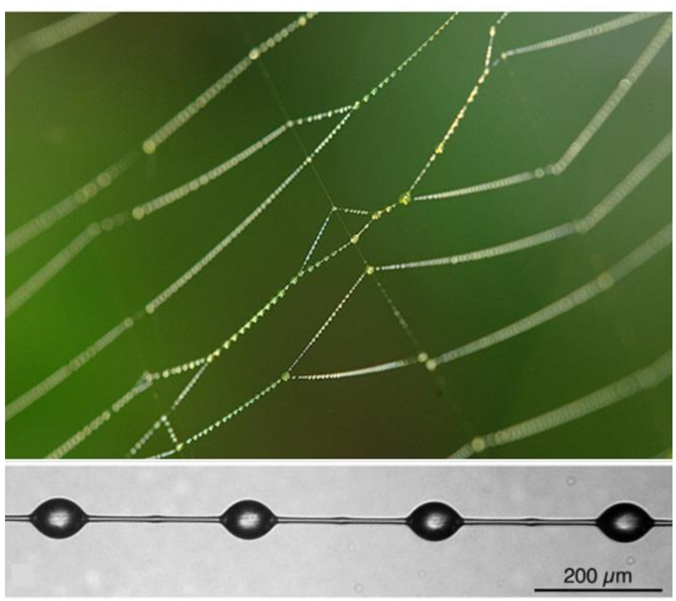

FIGURE 13

Orb-web weaving spider silk glue. (**A**) Photograph of aggregate glue droplets suspended on a web. (**B**) Microscopic image of aggregate gland glue droplets suspended on a flagelliform silk fiber from the *Larinioides cornutus* spider.

B. Modeling the Dynamics of Conflict and Cooperation within and between Multifarious Social Groups
Professor Sergey Gavrilets, University of Tennessee, Single Investigator Award

An ongoing challenge for the social sciences is predicting the conditions that lead individuals to contribute to the preservation of collective resources, such as a water or food supply. Such collective resources are fundamental to the survival of social organisms. Research shows that these resources tend to be distributed and maintained by social groups, which then require support from their members to protect them from other groups in order to ensure the intergenerational survival of the group. Yet, there is often an incentive to "free-ride" (i.e., reduce or eliminate any contribution of support, while still benefiting from the public good that others are supporting). If all group members take a free-ride, however, the survival of the group is put at risk. Conventional research has long assumed that the fewer free-riders there are in a group the greater the group's likelihood of survival. Thus the solution the free-rider problem is to ensure adequate costs for free-riding are imposed and incentives for contributions are offered. This creates an inefficient and costly system. Professor Gavrilets, however, has developed a counter-intuitive model to examine the free-rider problem through the study of non-human social species. This research shows that higher-status group members tend to usurp a larger proportion of collective resources and also exert greater contributions toward protecting those resources in between-group conflicts. Professor Gavrilets research shows that in non-human social species, greater within-group inequality will generate a greater total contribution to the preservation of collective resources. This is because the higher ranking group members, who benefit from a greater share of the resources, will contribute more toward protecting the resources as the benefits accrue (see FIGURE 14).

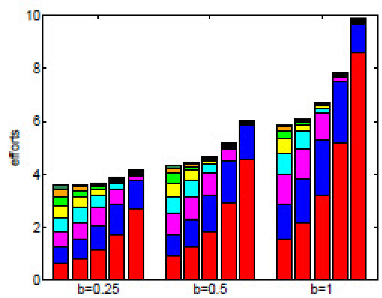

FIGURE 14

Efforts contributed to protect collective resources by benefit level and degree of status inequality. Colors show the contribution by group members of different status ranks, with the highest ranking individual shown in red at the bottom of the graph and the lowest ranking at the top. Each set of bars reflects a specific value of benefit and each bar stack within a set reflects different degrees of within-group inequality.

Another pathbreaking facet of Professor Gavrilets' model is that the relative contribution of higher status members grows as group inequality increases. As a consequence of their greater contributions toward protecting collective resources, higher status members are at greater risk, which suggests a greater decline in their reproductive fitness, due to increased morbidity and mortality (see FIGURE 15).

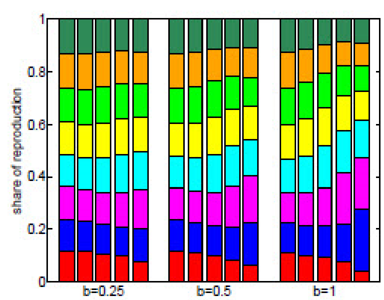

FIGURE 15

Reproductive fitness (share of reproduction) by benefit level and status inequality. Colors show the share of reproduction by group members of different status ranks, with the highest ranking individual shown in red at the bottom of the graph and the lowest ranking at the top. Each set of bars reflects a specific value of benefit and each bar stack within a set reflects a different degree of within-group status inequality.

In FY15, Dr. Gavrilets will expand these models to further using evolutionary game theory to model the evolution of social instincts corresponding to status ranks that govern individual behavior in social groups. Targeted behaviors in this phase of the project will include cooperation, competition, and punishment, as driven by selection, mutation, recombination, random genetic drift and migration.

C. Dynamic Network Neuroscience

Professor Danielle Bassett, University of Pennsylvania, Single Investigator Award

Cognitive processes that harness distributed networks of brain areas drive human behavior. For decades, the focus was to pinpoint brain region(s) associated with behavior. Emerging work shows this approach is flawed; the mammalian brain is constantly reconfiguring the relative connections among brain regions to enable learning, memory, and cognition. Rather than a static snapshot of brain function that may apply broadly to the population, it is clear that brain communication patterns are dynamic and are not described at all with current theoretical frameworks. The reconfiguration of brain activity and connectivity is particularly relevant to mission outcomes in the context of neural (and by extension behavioral) adaptation. Adaptation can be broadly defined as any alteration in the structure or function of an organism or any of its parts by which the organism becomes better fitted to survive and succeed in its environment. Long-term adaptation is a hallmark of learning, and therefore a common goal of training, either pre-mission outset or following mission-related injury. Shorter time-scale adaptations are particularly salient in military personnel in the form of cognitive flexibility to efficiently change a cognitive state or the ability to shift a decision criteria based on new and incoming information. These and related forms of adaptation enable a warrior to optimize his/her response to training, complex scenarios on the battle field, and rehabilitation following physical or psychological injury. Neural adaptation also plays a key role in soldier interactions with machine and computer interfaces, informing the use of these interfaces in combat and performance enhancement. Despite the mission relevance of neural adaptation, an understanding of these processes in large-scale brain circuitry has been hampered by the current lack of any approach to quantify, characterize, or predict these processes from non-invasive neuroimaging data in humans.

The goal of this multidisciplinary research is to develop “Dynamic Network Neuroscience” as a broadly applicable tool for probing adaptation of large-scale neural circuits. Building on proof-of-principle work, the investigator plans to extend those capabilities to examine changes in both activity and connectivity using novel activity connectivity representations which will be manipulated using non-invasive brain stimulation and neurofeedback in real-time fMRI under varying task demands.

It is anticipated that in FY14 a robust analytical method will be established to characterize structural and functional connectivity and predict the adaptation of neural circuits measured non-invasively in humans. The general approach begins with a functional magnetic resonance imaging (fMRI) scan acquired from a single human participant during a neural or behavioral adaptation process. Current efforts will be extended by developing summary statistics of brain network activity, test connectivity with statistical null models, and generate mechanistic models for combined activity-connectivity network representations of neuroimaging data acquired from a single human participant during a neural or behavioral adaptation process.

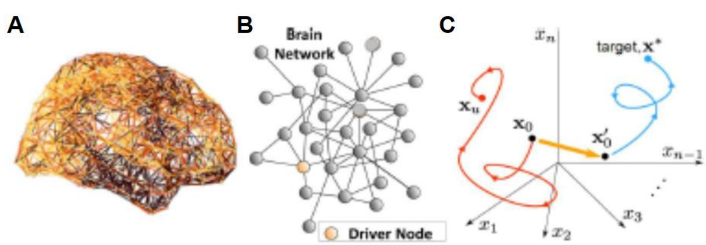

FIGURE 16

The approach of dynamic network neuroscience. A new approach here allows us to quantify, characterize, and predict the dynamics of regional activity and whole brain connectivity using a single mathematical framework and to link those dynamics to changes in behavior during cognitive processes accompanied by neural adaptation. First mechanistic models for adaptation of large-scale neural circuits from brain networks must be identified (**A**) and then they can be probed computationally to predicts changes to specific areas (**B**) and new mathematical tools can be incorporated to predict appropriate stimuli to move the system into new dynamic trajectories (**C**).

D. Forensic Palynology

Professor Vaughn Bryant, Texas A&M University, and Dr. Igor Pavlovsky, Applied Nanotech, SBIR Contract

Identifying the origin and recent history of people and materiel is a major technological challenge and critical to the success of current and future operations. One often needs to quickly know whether the person wanting to enter a sensitive area is who they say they are, or not. In addition, it would be useful to be able to verify their recent activities, such as travel to certain regions of the world. The rapid identification of pollen is an underutilized avenue for extracting information about a person's recent location and activities.

The objective of this research is to develop the capability to identify and characterize pollen obtained from mixed samples in an automated high-throughput system. There are four major characteristics of pollen that make it particularly informative: (i) Pollen is microscopic, generally ranging from 10-70 um in diameter. (ii) Pollen is abundant, being produced in vast abundance by male plants in order to fertilize female plants of the same species. As most pollen is generally dispersed by either wind or insects, the male plants must produce pollen in vast amounts (up to 100,000 grains of pollen per anther) to ensure that some of it will reach a female of the same species. (iii) Pollen is also very stable and has been identified in some cases after millions of years. (iv) Pollen is exceedingly complex and varies widely from species to species. (v) Pollen types are specific to time and place. A particular combination of pollen may enable the accurate identification where a human, body, computer, or other item has been, based on the variability in where plants can grow, when they produce pollen, how far a particular species of pollen can travel, and how stable a particular pollen is under specific conditions.

In close collaboration with forensic scientists in the Army and other government agencies, Drs. Vaugh and Pavlovsky are determining whether pollen identification can be automated by exploiting the volatile organic compound profile. The challenge has been that pollen identification is currently done by humans, training takes years, very few humans are trained palynologists, and even the most highly trained palynologist is still very slow. While pollen is already used in DoD and non-DoD forensics, current technological challenges prevent use of the information encoded in pollen in real time for DoD intelligence, security, and forensic applications. It is anticipated that in FY15 the investigators will finish their development of a prototype gas chromatography based system to identify pollen in an automated high throughput system. Scientists from the Defense Forensic Science Center and other agencies are planning a site visit in FY15 order to transition this developing technology as rapidly as possible. Real-time capabilities would greatly increase the ability of DoD and intelligence agencies to use the information embedded in pollen to rapidly track down terrorists and the source of other nefarious objects and personnel.

E. Not Different, Just Better: the Adaptive Evolution of an Enzyme

Professor Renwick Dobson, University of Canterbury, Single Investigator Award

While there has been a considerable body of research devoted to environmental adaptation on the organismal level, little is known about adaptation at the molecular level. One approach that can provide an understanding of the molecular determinants underlying adaptation is to identify and study enzyme variants that evolve under environmentally challenging growth conditions. To identify adaptive mutations that can confer improved function, Professor Renwick Dobson at the University of Canterbury in New Zealand is studying enzyme evolution in *E. coli* grown in a glucose-limiting environment. In twelve glucose-limited replicate bacterial populations grown out for 50,000 generations from a common ancestor, this group found that adaptive mutations are concentrated in relatively few genes. One of the genes containing an adaptive mutation in each of the 12 populations is *pykF*, which encodes pyruvate kinase (PK1), an enzyme that is central to the regulation of energy metabolism.

One PK1 variant that is common to three of the twelve populations contains a serine substituted for alanine at position 301 (A301S) of pyruvate kinase. When this variant replaces the chromosomal wild-type *pykF* gene in the ancestor strain, a 10-fold increase in fitness is observed. Further studies have shown that A301S is more thermally stable and exhibits better reaction kinetic than the wild-type enzyme. The crystal structure of this variant shows that the A301 S substitution is located at the tetrameric interface of pyruvate kinase. Interestingly, biophysical measurements of A301S have shown that, compared to the wild-type enzyme, there is more thermal motion in the presence of a critical allosteric effector at looped structures that are critical for substrate binding.

This increased flexibility of the A301S variant provides a molecular explanation for the improved enzyme kinetics.

In FY15, the Dobson group will study the intracellular and extracellular metabolomics of the A301S variant (and other PK1 variants) and perform metabolic flux analysis to comprehensively determine the metabolic advantages conferred by the adaptive *pykF* mutations. In addition, this group will investigate whether various PK1 variants are beneficial, neutral or deleterious in other resource-limiting environments. Collectively, completion of this analysis will provide a unique data set linking molecular- and organism-level phenotypes of a series of adaptive mutations.

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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 2014* is to provide information on the programs and basic research supported by ARO in fiscal year 2014 (FY14), and ARO's long-term vision for transitioning 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 FY14.

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 understanding 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. In addition to advancing and exploiting worldwide knowledge and understanding of new materials to achieve unprecedented properties, 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, Reliance 21 Community of Interest for Materials and Processes), 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.

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 FY14, the Division managed research within these four 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, magnetic and thermal properties in advanced materials to enable future Army relevant innovations. This Program Area is divided into two research Thrusts:

(i) Free-standing 2D Materials focuses on the creation of novel free-standing 2D materials, heterostructures and hybrids with physical properties complementary or superior to graphene, and the invention of novel characterization techniques specific to 2D materials to determine unprecedented properties.

(ii) Defect Science & Engineering explores the specific influence of defects (positive or negative) on the physical properties of novel functional materials, and elucidates defect control mechanisms during thin film growth and bulk processing of novel 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 nanocrystalline 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 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 FY14 were $64.9 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY14 ARO Core (BH57) program funding allotment for this Division was $7.0 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 $20.0 million to projects managed by the Division. The Division also managed $28.9 million of Defense Advanced Research Projects Agency (DARPA) programs, and $1.0 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $2.1 million for contracts. Finally, $5.9 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.8 million of 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 FY14 (*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 FY14 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 FY14, the Division awarded 24 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to investigate the use of virus-like particles (protein cages containing metallic clusters) as promising building blocks for the 3D self-organization of novel plasmonic materials, establish a quantitative and predictable knowledge base of the phenomena of room temperature magnetoelectric effect in thin films of hexaferrite materials, and establish design principles for structurally efficient nanostructured high entropy alloys with engineered phases and microstructures enabling strength and ductility values that exceed those of conventionally processed alloys. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Anna Balazs, University of Pittsburgh; *Four-dimensional Printing: Design, Assembly, and Modeling of Responsive, Temporally Programmable Materials*
- Professor Nikhilesh Chawla, Arizona State University; *Microstructural Design of Precipitate Strengthened Alloys with Enhanced Mechanical Properties - Experiments and Simulation*
- Professor Bogdan Dragnea, Indiana University at Bloomington; *Optical Interactions in Virus-Based Materials*
- Professor Chang-Beom Eom, University of Wisconsin - Madison; *Magnetoelectric Control of Exchange Bias Coupling in Monodomain Multiferroic Thin Film Heterostructures*
- Professor Mohammad Islam, Carnegie Mellon University; *Growth and Stability Nanocrystalline Domains within Three-Dimensional Carbon Nanotube Aerogels*
- Professor Roderic Lakes, University of Wisconsin - Madison; *Materials Created to Exhibit Extreme Physical Properties*
- Professor Enrique Lavernia, University of California - Davis; *Nanostructured High Entropy Alloys*
- Professor Xiaochun Li, University of California - Los Angeles; *Diffusional Growth Control and Stabilization of Nano-sized Minority Phase Using Nanoparticles in Bulk Immiscible Materials during Solidification*
- Professor Jonathan Malen, Carnegie Mellon University; *Non-equilibrium Phonon Transport in Free-standing 2D Graphene Heterostructures*

- Professor Nicholas Ouellette, Yale University; *Determining the Essential Elements of Hydrodynamic Erosion of Granular Beds*
- Professor Wounjhang Park, University of Colorado - Boulder; *Materials by Design*
- Professor Jonathan Parquette, Ohio State University; *Self-Assembly of Multifunctional, Adaptive Nanomaterials.*
- Professor Jay Perron, Massachusetts Institute of Technology (MIT); *Probing the Effects of Topography on Bedrock Fracture in the Shallow Subsurface*
- Professor Lisa Pfefferle, Yale University; *Copper Oxide (CuO) 2-D Nanosheets for Advanced Electronic and Optical Properties*
- Professor Shriram Ramanathan, Harvard University; *Structural and Electrical Properties of Metastable Oxide Phase Created Under Extreme Oxygen Pressures*
- Professor Shenqiang Ren, University of Kansas; *Organic Photovoltaic Multiferroics*
- Professor Richard Saykally, University of California - Berkeley; *Liquid Carbon, Glassy Carbon, and Their Surfaces*
- Professor Christopher Schuh, Massachusetts Institute of Technology (MIT); *Design of Stable Nanocrystalline Alloys in Compound-Forming Systems*
- Professor R. Sooryakumar, Ohio State University; *Magnetic Actuation of DNA-based Nano-Structured Materials*
- Professor Jonathan Spanier, Drexel University; *Vacancy-Enabled Nonlinear Optoelectronic Ferroelectric Semiconductors*
- Professor Yuri Suzuki, Stanford University; *Defect Engineering of Spin Polarized Transparent Conductors through Complex Oxide Epitaxy*
- Professor Norman Tolk, Vanderbilt University; *Depth-Dependent Defect Studies Using Coherent Acoustic Phonons*
- Professor Carmine Vittoria, Northeastern University; *Novel Epitaxial Films of Magnetoelectric Hexaferrite Materials*
- Professor Mingzhong Wu, Colorado State University - Ft. Collins; *Creation of Spin Voltages in Magnetic Thin Films upon Exposure to Light*

2. Short Term Innovative Research (STIR) Program. In FY14, the Division awarded 15 new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to predict the tensile properties of architecturally graded aluminum composites, understand the nature of chiral charge density waves (CDW) observed in certain materials with the aim of actively controlling and measure the chiral states of individual CDW domains, and characterize the dynamics of colloidal binder (i.e. ink) interactions with three dimensional structures. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Jennifer Carter, Case Western Reserve University; *Interface Effects of The Properties And Processing of Graded Composite Aluminum Alloys*
- Professor Yury Gogotsi, Drexel University; Measurement of Mechanical/Elastic Properties of a Monolayer and/or a Few Layers of Different Mxenes
- Professor Maria Iavarone, Temple University; *Manipulation of Chiral Charge Density Waves*
- Professor David Lipke, Alfred University; Selective Metallothermal Reactions for Ceramic Matrix Nanocomposites
- Professor Ronghui Ma, University of Maryland - Baltimore County; *Computational Study of Colloidal Droplet Interactions with Three Dimensional Structures*
- Professor Jon-Paul Maria, North Carolina State University; *Fundamental Property Measurements of Entropy Stabilized Oxides*
- Professor Amiya Mukherjee, University of California - Davis; *An Investigation on the Mechanical Behavior of Roll-Bonded Multilayered Cu-Nb Nanocrystalline Materials*
- Professor Bart Raeymaekers, University of Utah; *Scalable Directed Self-Assembly Using Ultrasound Waves*

- Professor Rishi Raj, University of Colorado - Boulder; *Unusual Phase Transformations in Ceramics and Related Materials Under the Influence of an Electric Field*
- Professor Christopher Saldana, Pennsylvania State University; *Multi-scale Texturing of Metallic Surfaces for High Performance Military Systems*
- Professor Surajit Sen, State University of New York (SUNY) at Buffalo; *Stable Intrinsic Localized Modes in Microelectromechanical Cantilever Structures*
- Professor Moneesh Upmanyu, Northeastern University; *Enhanced Stability and Mechanics of Ultra-fine Grained Metals via Engineered Solute Segregation*
- Professor Xudong Wang, University of Wisconsin - Madison; *Growth of Large-Area, Free-Standing, Ultrathin 2D Nanomaterials at Solution Interface*
- Professor Yue Wu, University of North Carolina - Chapel Hill; *Disordered Layered Materials with Magnetization Oscillations*
- Professor Nicole Zacharia, University of Akron; *Polyelectrolyte Based Mechano-Responsive Materials for Energy Dissipation*

3. Young Investigator Program (YIP). In FY14, the Division awarded two new YIP projects. These grants are driving fundamental research, such as studies to establish a computational capability for designing metamaterials with user-defined thermal radiative properties and develop complete understanding of the structure-property relationships that dictate electron transfer at organic-inorganic interfaces and introduce a new paradigm for controlling electron transfer at hybrid interfaces.. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor Mathieu Francoeur, University of Utah; *Design of Thermal Metamaterials Beyond the Effective Medium Theory*
- Professor Kenneth Hanson, Florida State University; *Asymmetric Electron Transfer Rates At Organic-Inorganic Hybrid Interfaces Via Self-Assembled Bilayers*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY14 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *2013 Materials Research Society (MRS) Fall Meeting*, Boston, MA, 2-6 December 2013
- *2014 Materials Research Society (MRS) Spring Meeting*; San Francisco, CA; 21-25 April 2014
- *2014 Bioinspired Materials GRC and GRS*; Newry, ME; 22-27 June 2014
- *US-Europe Workshop on Impact of Multifunctionality on Damage Evolution in Composite Materials*; Seville, Spain; 25-26 June 2014
- *2014 Solid State Studies in ceramics: Transport and Reactivity GRC and GRS*; South Hadley, MA; 20-25 July 2014
- *Pan American Materials Conference*; Sao Paulo, Brazil; 21-25 July 2014
- *2014 Defects in Semiconductors GRC and GRS*; Waltham, MA; 3-8 August 2014
- *Technical Exchange on 2D Atomic Sheets: Optoelectronics, Strain, and Energy Applications*; Adelphi, MD; 12-13 August 2014
- *Third International Symposium on Phase-field Method*; State College, PA; 26-29 August 2014
- *18th International Conference of the International Society for Terrain Vehicle Systems, Seoul, Soth Korea*; 22-25 September 2014

5. Special Programs. In FY14, 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 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. Materials on the Brink: Unprecedented Transforming Materials. This MURI began in FY07 and was granted to a team led by Professor Kaushik Bhattacharya at the California Institute of Technology. The objective of this research is to develop a fundamental understanding and establish the engineering expertise needed to tailor the electrical, optical, or magnetic (EMO) properties of phase transforming materials through the design and implementation of highly reversible, phase-transformations.

This research is investigating different approaches to achieving highly reversible phase transformations, including such effects as engineered phase compatibility and frustration. The broad selection of material systems (perovskites and multi-ferroics, Heusler alloys, SMA, and oxy-acid proton conductors), and the design of the studies, will develop a fundamental understanding of the underlying physics that developers need to predict the occurrence of states and the range of behaviors that can be realized within engineered phase transforming materials. The specific goals of this project are to develop and characterize (i) perovskites for electrically tunable photonics and RF-to-optical converters, (ii) metal-ferroelectric multilayers for negative refractive index material applications (a negative surface-plasmon polariton was shown to provide NIM behavior in the visible part of the spectrum), light modulators, thermo-magnetic cooling, spintronics and magnetic field sensing, (iii) shape-memory alloys for large-strain actuators, and (iv) proton-conducting electrolytes for fuel cells. New strategies based on phase engineering of materials have been successfully realized in actuation systems (*e.g.*, in shape memory alloys and relaxor ferroelectrics). These same underlying principles may ultimately be transferable to the development of EM sensors, tunable phase shifters, adaptive optics, optical limiting and energy harvesting devices for use by the Army.

2. Electrical Control of Magnetic Dynamics in Hybrid Metal-Semiconductor Systems. This MURI began in FY08 and was granted to a research team led by Professor Daniel Ralph at Cornell University. The objective of this research is to investigate fundamental phenomena that will enable the all-electrical manipulation of magnetic behavior (both static and dynamic properties) in hybrid structures incorporating magnetic metals, multiferroic oxides and semiconductors.

This research involves fundamental studies on spin injection and transport studies in hybrid metal-semiconductor systems and establish the materials growth and nanofabrication techniques needed to develop a new class of hybrid spin-based electronics. Five studies are being pursued: (i) to study spin injection across metal-semiconductor interfaces, (ii) to develop spin-transfer-torque oscillators and switches, (iii) to pursue the integration of multiferroic materials for electric-field control of exchange coupling bias, (iv) to investigate general approaches to electrical manipulation of spins (electron and nuclear spins), and finally (v) to identify electrical approaches to manipulation of coupled spins in diamond. One key goal is to obtain three orders of increase in the current density of injected spin polarized currents across metal-semiconductor interfaces.

3. Spin-Mediated Coupling in Hybrid Magnetic, Organic, and Oxide Structures and Devices. This MURI began in FY08 and was granted to a team led by Professor Michael Flatte at the University of Iowa. The objective of this research is to investigate fundamental spin-based properties of novel hybrid structures incorporating magnetic metals, multiferroic oxides and organic semiconductors.

This research seeks to develop a new class of hybrid magneto-electronics that can move towards the seamless integration of memory and logic functions under a single device format. The research will conduct some very fundamental studies on spin injection and transport studies in hybrid metal-organic systems. In addition, this work will also look at aspects of nuclear spin imprinting in organics, spin-wave guiding, GHz spin precession and phase locking of sources, OLED modulation, electric-field tuning of spin injection from multiferroic contacts, and electrical switching of ferromagnetism in quasi 2DEG oxide heterostructures. Pioneering studies on magnetoresistance (OMAR) and nuclear spin polarization in organic systems and on conductor-insulator induced transitions in the magnetism of 2DEG oxide heterostructures ($SrTiO_3$ and $LaTiO_3$) are being conducted. It also proposes a very interesting task to use organic overlayers to image the evolution of spin waves from metallic spin torque devices. The program includes a significant theory and modeling task to help guide the experimental effort. As the material capabilities become better defined the program will seek to identify and prototype new device structures relevant to applications in sensors, magnetic storage, dynamic memory and logic, and spin-wave mediated data transfer.

4. Design of Adaptive Load Mitigating Materials Using Nonlinear Stress Wave Tailoring. This MURI began in FY09 and was granted to a team led by Professor John Lambros at the University of Illinois, Urbana. This research is focused on understanding and exploiting wave tailoring phenomena in highly nonlinear inhomogeneous granular media.

The effort builds on recent results demonstrating remarkable dynamic properties in such media, including tunability, energy trapping and wave redirection, primarily because of the highly nonlinear forces that are generated during contact of the granular crystals. Specific granular microstructures will be designed to fully exploit the nonlinear contact effect. Additionally, novel phase transforming ceramics will be fabricated that enhance the granular materials properties by, for example, preferentially strengthening or weakening the material to control local energy dissipation. The specific goals of this research are to (i) incorporate a granular medium in the material system in order to introduce nonlinearity in the material microstructure through local contact between material "elements", thereby furnishing an adaptive and nonlinear targeted energy transfer (TET) capability, (ii) provide additional adaptively coupled with enhanced energy absorption by developing new phase transforming ceramics, (iii) arrange these and other elements in a material system that is either layered (2D), or integrated with a 3D microstructural architecture, and (iv) utilize geopolymers (polymer-like ceramics) to create interfaces that join constituents and also act as "traditional" wave arrestors or reflectors. The comprehensive understanding of propagation and mitigation of high-pressure stress-waves in complex media will guide the future design and demonstration of new materials optimized for high-strain-rate ballistic performance, particularly armor materials. The research is expected to ultimately enable lightweight military hardware with dramatically enhanced survivability, in addition to new paradigms for insensitive munitions.

5. 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

6. 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.

7. **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.

8. **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.

9. **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.

10. **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.

11. 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.

12. Multiscale Mathematical Modeling and Design Realization of Novel 2 D 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.

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

No new starts were initiated in FY14.

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 FY14, the Division managed six new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of five Phase I contracts and one 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 FY14, the Division managed two new ARO (Core) HBCU/MI projects and 14 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 PECASE winners for each calendar year are typically announced by the White House at the end of the fiscal year. However, the 2014 PECASE recipients had not yet been announced at the time this issue of ARO in Review was completed. 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 FY14, the Division managed six 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 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 Advanced Structural Fiber (ASF) Program

The goal of the ASF program is to develop and produce a fiber that offers at least a 50% increase in strength and stiffness. The ASF program is focused on exploiting recent breakthroughs in the understanding of materials synthesis at the atomic level, new materials characterization techniques, and advanced fiber manufacturing processes to scale up production fiber technologies that have already shown revolutionary lab-scale results. The Division currently co-manages projects within this program seeking to explore and optimize the most promising fiber compositions and processing strategies and to establish new paradigms for revolutionary fiber precursors.

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 ARO Materials Science 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.

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. New Jamming Phenomena Revealed in Sediment Transport

Professor Douglas Jerolmack, University of Pennsylvania, Single Investigator Award

The objective of this research is to develop a granular physics approach to understanding fluid-driven sediment transport. In FY14, researchers at the University of Pennsylvania constructed a unique experimental apparatus to examine laminar bed-load transport that employs (1) refractive-index matching and laser scanning to provide 3D tomography of a mobile granular bed, (2) vibration isolation and control to minimize experimental noise, and (3) newly developed particle tracking algorithms. Data from recent experiments have allowed the determination of particle velocity over six orders of magnitude from thousands of particle trajectories. Major findings are that the particle velocity profile exhibits a double exponential form consisting of an upper "fluid-like" layer, and that this profile transitions below the surface to quasi-static behavior (see FIGURE 1). This transition occurs at a critical inertial number, consistent with recent observations in dry sheared granular flows and colloidal suspensions, and strongly suggests that the onset of bed-load transport is a granular jamming transition.

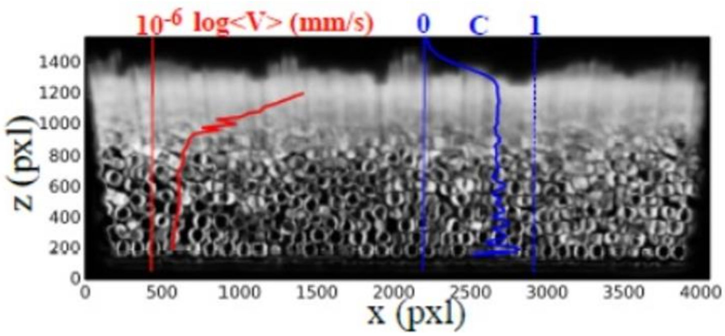

FIGURE 1

Particle tracking results. Image of the standard deviation at each pixel over a 10-hour experiment showing an active upper layer (blurred) and a slowly moving layer underneath. Blue and red curves represent, respectively, the long-term averaged particle concentration and velocity.

B. High Energy-Product Permanent Magnets Using Cobalt Nanowires

Professor J. Ping Liu, University of Texas - Arlington , Single Investigator Award

The objective of this research is to investigate the fundamental aspects and processing approaches relevant to the development of hybrid magnets with superior properties. In FY14, the research team demonstrated that pure cobalt nanowires can be used to prepare high energy-product permanent magnets that will enable an integrated magnetic capability for future advanced communications and targeting systems. Cobalt nanowires with a high aspect ratio were synthesized using a solvothermal chemical process and then epoxy bonded to produce an aligned nanowire composite that displayed surprisingly high coercivity. The resulting high coercivity may ultimately lead to energy products as high as 44 MGOe, depending on the inal density of the composites.

This discovery may surpass all commercially-available magnets except for the neodymium magnets that are of little utility to the DoD because of their relatively low maximum operating temperature. This breakthrough represents the first critical step in the development of a new generation of rare-earth element-free hard magnetic materials. An added advantage of this class of magnet is that they will have good high thermal stability and oxidation resistance which should permit operation at temperatures far above those of current magnets.

C. Electric Fields Accelerate Densification of Ionic Ceramics

Professor Klaus van Benthem, University of California - Davis, Single Investigator Award

The objective of the research is to evaluate the fundamental mechanisms by which electrical fields can enable the accelerated consolidation of materials during field assisted sintering. In FY14, researchers at the University of California - Davis performed in situ heating experiments using transmission electron microscopy (TEM) to directly observe particle agglomerates during sintering. Electric field assisted sintering was employed to separate the effect of temperature and electrical field strength on green bodies. A new micro-electromechanical systems (MEMS) device was developed (see FIGURE 2), and 3YSZ nanoparticles were drop-cast onto the MEMS device to perform the first systematic experiments to evaluate the role of an electrostatic field during (flash) sintering. Data indicate that electrical fields at or above 500V/com accelerate densification at temperatures 100-200K below typical densification temperatures (see FIGURE 3).

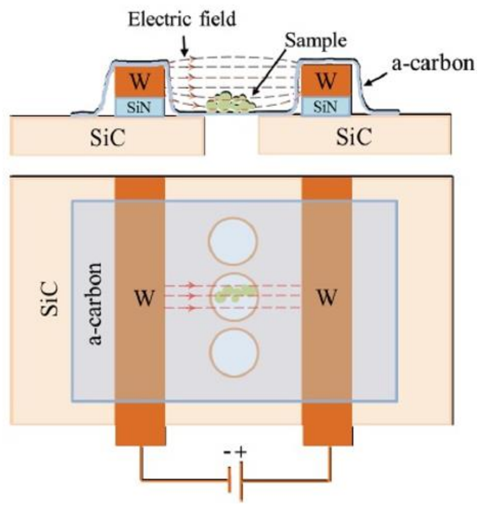

FIGURE 2

Sketch of electro-thermal MEMS device used for in situ TEM experiments. The device consists of a monolithic silicon chip onto which a SiC heating membrane and two tungsten electrodes are placed to control sample temperature and apply an electrostatic field to the sample, respectively. The electrodes are electrically separated from the SiC membrane by SiN dielectric layers.

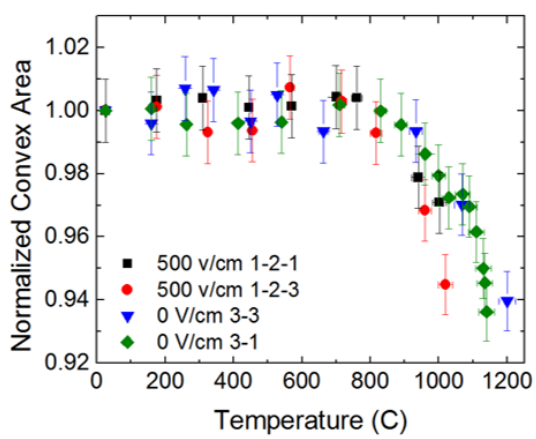

FIGURE 3

Densification curves for 3YSZ particle agglomerates. Data are from from in situ TEM experiments with and without the allocation of an electrostatic field strength of 500V/cm; curves were obtained using a previously developed image processing algorithm.

D. Catalysis at Strained Surface Steps: Mechanical Energies Dominate
Professor Pradeep Guduru, Brown University, MURI Award

The objective of this research is to develop a scientific basis for controlling and manipulating catalytic reactions using applied stress. In FY14, researchers at Brown University demonstrated that catalysis at strained surface steps is dominated by mechanical energies. This result led to the discovery of a new and unexpected phenomenon: mechanical relaxation occurring in surface steps during chemisorption causes a reversal of the "tension strengthens binding" trend for late transition metals (LTM) stepped surfaces. This discovery can be used to tune and enhance catalytic activity and suggests a new engineering principle for the control/modulation of catalytic reactions through the application of mechanical strain. Such strain may result from an applied stress or be induced by a lattice mismatch, as in pseudomorphic layers and core/shell nanoparticles. This phenomenon was explored through the application of mechanical strain to enhance the methanation reaction on Ni, in which the catalytic activity scales with the dissociation energy of the CO molecule. A major finding is that that opposing trends in chemisorption energy versus strain on the same substrate can have a significant influence on catalytic activity and transform sub-optimal materials such as Ni into peak-performing materials (see FIGURE 4).

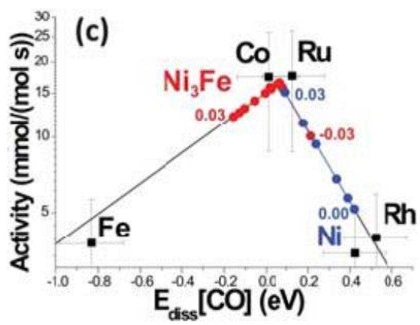

FIGURE 4

Methanation activity versus dissociation energy of CO. Black lines are computed values from the literature; solid squares are experimental/computational results on unstrained Ni, Rh, Ru, Co, and Fe from the literature; blue and red circles are current predictions for Ni and Ni_3Fe, respectively, under biaxial strain in steps of 0.5%. Note that an increase in biaxial strain of 3% in Ni can increase the predicted and measured activity of Ni to its maximum. Strain can thereby make the suboptimal catalyst Ni optimal and shift the activity of Ni to be equal to that of Co or Ru.

E. Understanding the Scientific Basis of Electrocaloric Effect In Defects Modified Ferroelectric Polymers
Professor Theodore Goodson, University of Michigan, Single Investigator Award

This research aims to develop scientific basis and understanding of the electrocaloric effect (ECE) in defects modified ferroelectrics. ECE is directly related to the dipolar entropy difference between a dipole ordered and disordered states in dielectric materials, especially ferroelectric materials, which can be switched by external electric fields. Defects structures play critical role in influencing the dipole ordering and energy balance among different states of dipole ordering. The scientific accomplishments of this project include scientific understanding on how various defects structures influence the polarization responses at high electric fields.

In FY14, the PI demonstrated that besides the defects at the atomic level (such as in the bulky monomers R in the P(VDF-TrFE-R) terpolymer and crosslinking with bulky pedant groups in the high energy irradiated P(VDF-TrFE) copolymers), the nano-scale defects structures such as interfaces can also significantly alter or even enhance the EC responses. Better scientific understanding has led to the development of a totally new concept in enhancing the ECE, that is, the invariant critical point (ICP) in ferroelectric materials, which maximize the coexisting phases and near which the energy barriers for the switching among these phases become vanishingly small. Experimental demonstration of an ICP material systems, the $Ba(Ti_{1-x}Zr_x)O_3$ system, where the combination of ICP, relaxor response, and the substrate coupling result in a giant ECE, (see FIGURE 5), which is the highest ECE (>2 X compared with all the other results) reported in the literature in bulk ceramics.

More excitingly, by tuning the defects coupling in the blends of normal ferroelectric P(VDF-TrFE) and relaxor terpolymer P(VDF-TrFE-CFE), The PI has discovered an anomalous ECE. That is, the dielectric material will cool under an electric pulse, whereas in normal ECE, applying an electric field to a dielectric material will cause heating and removing the field will cause cooling (see FIGURE 6). This is similar to the vapor cycle cooling: applying pressure to the refrigerant gas causes heating and expanding the refrigerant gas causes cooling). The discovery of the anomalous ECE opens up a totally new ECE research direction as well as new applications. The development of high efficiency, compact, and high cooling power cooling systems will have impact on electronics cooling for Army where smaller sizes and increased functionality have resulted in higher power densities and thus significant increases in the heat generated at the component, board and system level. It will also impact on the thermal management of soldiers in the battlefield wearing chemical protective gears.

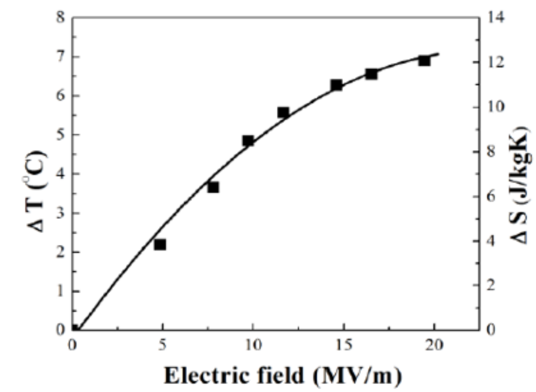

FIGURE 5

EC-induced temperature drop ΔT and isothermal entropy change ΔS for the different electric fields at 40 °C for BZT at x=0.2.

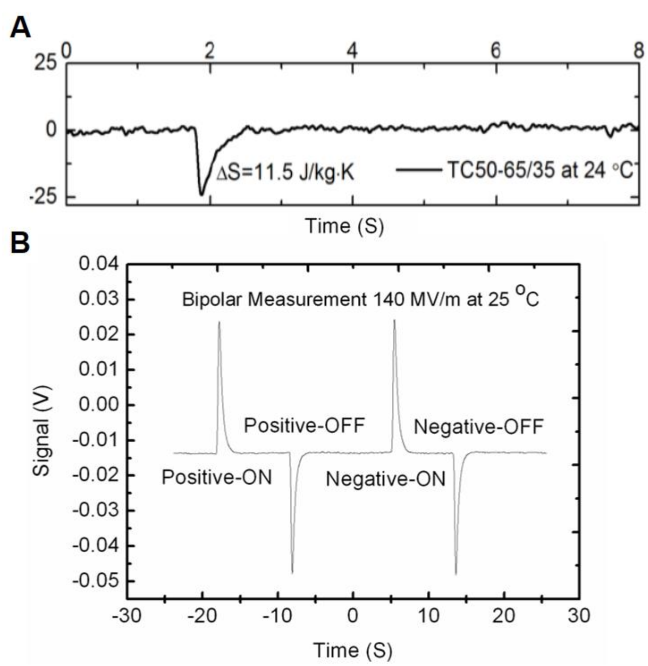

FIGURE 6

Anomalous ECE, whereby the dielectric material cools under an electric pulse. (**A**) the anomalous ECE which has cooling peak only under the application of an electric pulse (applying a field and then reducing to field to zero); (**B**) the normal ECE where applying a field causes heating (positive peak) and removing field causes cooling (negative peak)

F. Resonant Light Sorting of Microspheres
Professor Vasily Astratov at the University of North Carolina - Charlotte, Single Investigator Award

The objective of this research program is to develop new high throughput techniques for selecting groups of supermonodispersive microspheres, self-organizing into closely spaced 3D arrays, and finally investigating the mechanisms of optical coupling and wave propagation in resonant optical circuits composed of arrays of these nearly identical microresonators. In FY14, the research team demonstrated that light transmitted down a tapered fiber, when tuned to the resonance (e.g. whispering gallery) mode of a nearby polystyrene microsphere, can lead to strong radial trapping of the sphere near the tapered fiber and then propulsion along the length of a tapered fiber in the direction of the propagating light. While the response for 10 micron spheres was quite weak, the coupling for spherical particles 20 microns or larger in size was very strong (see FIGURE 7). Under near resonance conditions the 20 um particles were found to acquire significant velocity (up to 16 um/s mW) along the beam direction. The propulsion forces coincided precisely with the measured profiles of the whispering gallery mode resonances of the microspheres. This technique suggests a unique way of achieving large-volume sorting of nearly identical photonic particles with exception uniformities on the order of $1/Q$, where Q is the resonance quality factor of the sphere. This represents an enabling technology for developing super low-loss coupled-cavity structures and devices.

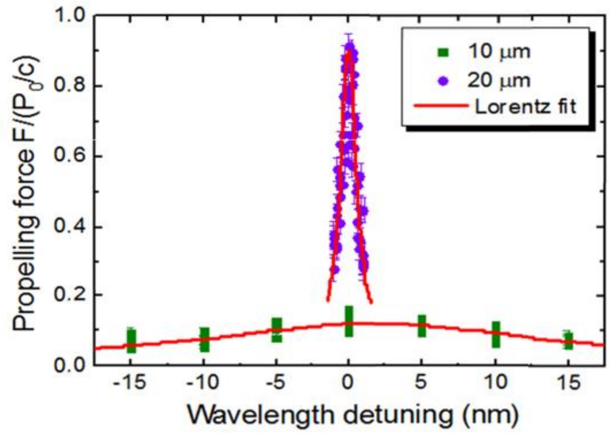

FIGURE 7

Force exerted on polystyrene microspheresas a function of laser detuning from the central resonance of the sphere.

G. Disordered Layered Materials with Magnetization Oscillations
Professor Yue Wu, University of North Carolina - Chapel Hill, STIR Award

The objectives of this research are to synthesize novel amorphous activated carbon materials with local structures exhibiting graphene like characteristics, explore novel methods to characterize them, and explore the effects of defects on electronic/magnetic properties in these materials. Ion distribution in aqueous electrolytes near the interface plays critical roles in electrochemical, biological and colloidal systems and is expected to be particularly significant inside nanoconfined regions. Electroneutrality of the total charge inside nanoconfined regions is commonly assumed *a priori* in solving ion distribution of aqueous electrolytes nanoconfined by uncharged hydrophobic surfaces with no direct experimental validation. In FY14, the PI used a quantitative nuclear magnetic resonance to investigate the properties of aqueous electrolytes nanoconfined in graphitic-like nanoporous carbon prepared in his lab. He observed substantial electroneutrality breakdown in nanoconfined regions and very asymmetric responses of cations and anions to the charging of nanoconfining surfaces. The electroneutrality breakdown is shown to depend strongly on the propensity of anions toward the water-carbon interface and such ion-specific response follows generally the anion ranking of the Hofmeister series. The experimental observations are further supported by numerical evaluation using the generalized Poisson-Boltzmann equation in this work.

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 to external organizations and customers.

A. Spin-transfer Torque Switching of Magnetic Devices

Investigator: Professor Daniel Ralph, Cornell University, Single Investigator Award
Recipients: IBM, Hitachi Global Storage Technologies, Qualcomm, Samsung, and Intel

For the past five years researchers at Cornell University have been conducting ground breaking studies on the switching of magnetic tunnel junction devices using spin-transfer torque techniques. Initially, their studies focused on using spin-polarized currents produced by flowing currents through magnetic contacts. However, this approach is inherently limited in spin flip efficiency (one flip per electron).

Recent breakthroughs at Cornell have discovered that spin-torque efficiencies and damping coefficients can be improved by orders of magnitude by incorporating materials with strong spin-orbit interactions which can be introduced using heavy-metal / ferromagnet bilayers and topological insulator / ferromagnet structures (see FIGURE 8). Not only are these much more efficient (multiple flips per electron), spin torque currents arising from spin-orbit interactions (spin-Hall effects) can be used with a much broader range of magnetic materials, including insulators, since the spin torque is directed perpendicular to the applied charge current, see figure. This breakthrough opens the possibility of incorporating insulating antiferromagnetic materials into the device structures, potentially leading to much higher operating frequencies and significantly lower intrinsic damping. The Cornell team has been collaborating directly with researchers at IBM, Hitachi Global Storage Technologies. Qualcomm, Samsung, and Intel to develop spin-torque magnetic random access memory and high frequency resonators based on the principles of spin-transfer torque.

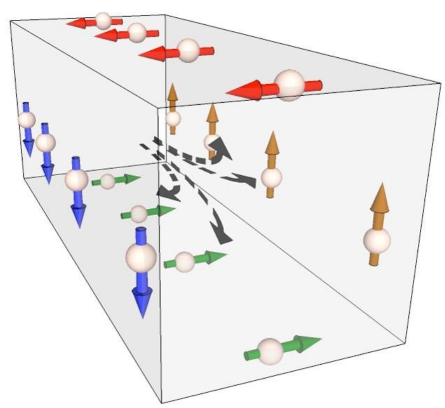

FIGURE 8

Spin-orbital scattering of a current in a heavy metal (e.g. Pt or W) will generate radial spin polarized current flow perpendicular to the current flow direction.

B. Enhanced Water Transport in Novel Anion Exchange Membranes

Investigator: Professor Andrew Herring, Colorado School of Mines, MURI Award
Recipient: Natick Soldier Research Design and Engineering Command (NSRDEC)

The objective of the ongoing research is to produce revolutionary, robust, durable, thin anion exchange membranes and to improve understanding of the interplay of chemistry, processing, and morphology governing their performance and durability. In FY14, three durable anion exchange membranes were sent to researchers at NSRDEC where they are analyzing the water vapor flux through the films as a function of vapor activity. Preliminary results have demonstrated exceptional water vapor flux, in addition to excellent water transport over a range of temperatures. The characteristic solubility parameters and diffusion coefficients have also been determined, and preliminary characterization of the transport of alcohols has been performed.

C. Characterizing the Effects of Blast Injury on Neuronal Tissue and Circuits
Investigator: Professor David Meaney, University of Pennsylvania, MURI Award
Recipient: ARL Weapons and Materials Research Directorate (ARL-WMRD)

The objectives of the research effort are to define how blast is transferred to the brain at multiple length scales (synapse-dendrite-neuron circuit), to determine when blast causes structural and functional changes at these length scales, to measure how multiscale alterations are linked and extend into neurobehavior, and to develop valid scaling principles. In FY14, joint research efforts were initiated with researchers at ARL-WMRD to develop novel experimental facilities to characterize the effects of blast impact on neuronal tissue in vitro, to simulate blast wave impact effects on living tissues, and to develop a valid coarse-grained molecular dynamics simulation of structural changes in lipid membrane due to shock waves. The collaborations are extending the frontiers of science in each of these areas and providing unique capabilities within ARL-WMRD to conduct future research.

D. Atomic Layers of Nitrides, Oxides, and Sulfides (ALNOS)
Investigator: Professor Pullickel Ajayan, Rice University, MURI Award
Recipients: ARL-SEDD and ARDEC

This MURI project focuses on developing fundamental science of two dimensional (2D) atomic layers of nitride, oxide and sulfide materials. The MURI team has successfully worked on a large number of 2D systems, on a variety of aspects such as scalable synthesis, defect engineering, atomic scale characterization and understanding electronic transport. Over the past three years, the team has worked together, from both theoretical and experimental aspects, to address some of the main basic science challenges that are at the core of the project. As part of this, the team has established strong collaboration with DoD laboratories in particular, ARL-SEDD and AREDC. Scientists from DoD labs (ARL Adelphi and AFRL Dayton) have visited Rice University to learn the vapor phase growth of some of the transition metal dichalcogenide (TMD) layers such as MoS_2. ARL-SEDD and ARDEC scientists have worked on the TMD samples produced by the MURI team, to explore the Raman and Photoluminescent (PL) spectroscopic features in these samples and transport measurements that would elucidate the role of defects and grain boundaries on electrical transport. ARL-SEDD scientists also worked closely with the MURI team to try and solve the issue of contacts on monolayer WS/Se_2. A graduate student from Penn State University worked at ARL-SEDD for few months and another student from Rice University has joined the group at ARL-SEDD as a post-doctoral fellow to continue the work. These collaborations and tech-transfer have resulted in several peer reviewed publications co-authored by MURI team members and ARL scientists.

A number of excellent results have been obtained from these collaborations. Understanding the role of defects in these 2D atomic layers has been key to further improve the quality of the samples and build useful structure-property correlations. Raman and PL have been extensively used to understand the structural features in these layers as well as determine the signature from various TMD compositions. For example, a blue shift in the excitonic peak and an increase in the PL quantum yield were observed for the first time when the MoS_2 layer was folded and this result is contrary to expectations. State of the art facilities available at the sites of the MURI team members and at ARL have been synergistically used to get the best results, in particular for characterization and transport measurements. Systematic work has shown the possibility of bandgap engineering in these 2D layers using strain engineering and this is expected to benefit future application of these materials in flexible electronics. The influence of substrates on the performance of these 2D layers is yet another area that has been explored in these collaborations. In summary, the close collaboration with ARL-SEDD and ARDEC scientists and the MURI team has enabled significant progress in the field and could lead to applications that are relevant to DoD missions in the future.

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. Jamming by Design in Soft Matter

Professor Heinrich Jaeger, University of Chicago, Single Investigator Award

The objective of this research is to investigate the role of local, particle-scale properties in affecting the overall response to applied stresses as the jamming transition is crossed. More specifically, the effort broadly seeks to extend the current understanding of the jamming transition by focusing on aspects that allow for control of the dynamic interactions among particles, in particular particle shape and interstitial fluids. Recent breakthroughs have identified particular opportunities in soft matter to manifest a robust jamming transition. In FY15, the research will demonstrate disordered, amorphous systems to switch reversibly between solid-like rigidity and fluid-like plasticity, and enable materials that can change stiffness and shape adaptively.

B. Luminescence Dating With Record Short Timescales

Professors Edward Rhodes, University of California - Los Angeles, STIR Award

The objective of this research is to assess the potential of applying dating methods based on natural mineral luminescence of common surface minerals such as quartz and feldspar for short-term dating of heating and burial events. These techniques, optically stimulated luminescence and infrared stimulated luminescence, are typically used to date events occurring at least hundreds of years in the past. The PI will reduce the minimum resolvable radiation dose through a combined approach involving instrumental modification and calibration, use of high-sensitivity materials and technique optimization. It is anticipated that in FY15, the PI will develop a reproducible technique for dating heated structures at the shortest time scales ever recorded, using common earth surface materials.

C. Asymmetric Electron Transfer Rates At Organic-Inorganic Hybrid Interfaces Via Self-Assembled Bilayers

Professors Kenneth Hanson, Florida State University, Young Investigator Program (YIP) Award

The objective of this proposal is to develop a basic understanding of structure-property relationships that dictate electron transfer at organic-inorganic interfaces and introduce a new paradigm for controlling electron transfer at hybrid interfaces. To achieve this objective, the PI proposes to generate two classes of rectifier-like molecules and incorporate them into self-assembled bi-layer films. These films will be used as a spectroscopic platform to probe electron transfer rates at hybrid interfaces. It is anticipated that in FY15, deliverables from this project will include: (1) a new scaffolding to study single molecule rectifiers, (2) a library of bridging molecules capable of asymmetrically influencing electron transfer dynamics, and (3) improved understanding of how the bridges structure-property relationship influences electron transfer rates/mechanism at hybrid interfaces. If successful, the findings of this work are anticipated to aid in the rational-design of hybrid interfaces that optimize electron transfer dynamics which can be directly applied in bio/organic electronics, solar energy conversion, electrocatalysis, sensing and other applications etc.

D. Principles of Colloidal Self Assembly

Professor Sharon Glotzer, University of Michigan, MURI Award

A team of researchers headed by Professor Sharon Glotzer at the University of Michigan are seeking to understand the self-assembly of complex building blocks characterized by patchy interactions. Using lock-and-key colloids as a model system, Glotzer is conducting a series of complementary theoretical and experimental studies to gain fundamental new insights on how patchy particles bind and self assembly into larger structures..

The lock-and-key colloidal particles consist of a central spherical colloidal particle (key) attached to a finite number of dimpled colloidal particles (locks) via depletion interactions strong enough to bind the particles together but weak enough that the locks are free to rotate around the key. This rotation imbues a mechanical reconfigurability to these colloidal "molecules" that allows them to anneal out of kinetic traps and reach final configurations that they would not otherwise be able to access. Initial molecular simulations predict that these lock-and-key building blocks can self-assemble into a wide array of complex crystalline structures that are tunable via a set of reconfigurability parameters, including: the number of locks per building block, bond length, size ratio, confinement, and lock mobility (see FIGURE 9). These simulations have shown that non-specific binding is a key feature in enabling the assemblies to reach specific targeted binding configurations. Complementary experimental studies are underway to confirm these findings. In FY15, this work is expected to guide appropriate selection of complex building blocks that can self-assemble into their thermodynamic ground state with good fidelity; or conversely indicate that certain specific targeted structures are too complex and therefore that more aggressive methods such as field-assisted or shear-assisted assembly will need to be used.

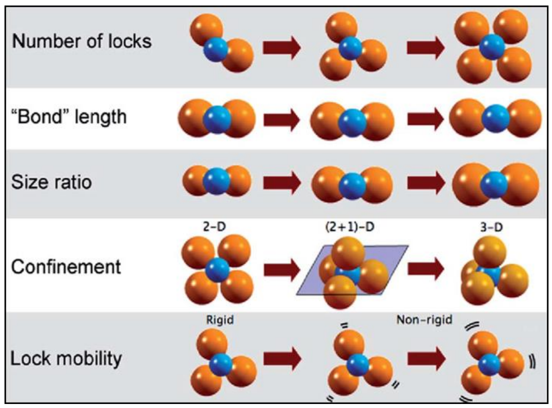

FIGURE 9

Parameters influencing the reconfigurability of bonding during the self-assembly process.

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
Program Manager (Acting), Earth Materials and Processes

Dr. John Prater
Program Manager, Materials Design

Dr. Chakrapani (Pani) Varanasi
Program Manager, Physical Properties of Materials

Dr. Julia Barzyk
Contract Support, Earth Materials and Processes

B. Directorate Scientists

Dr. Thomas Doligalski
Director, Engineering Sciences Directorate

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. Pamela Robinson
Administrative Support Assistant

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 2014* is to provide information on the programs and basic research supported by ARO in fiscal year 2014 (FY14), and ARO's long-term vision for transitioning 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 FY14.

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. In addition to advancing global knowledge and understanding of mathematical concepts, structures, and algorithms, the research managed in 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 Army scientists and engineers, such as the ARL Weapons and Materials Research Directorate (ARL-WMRD) and ARL Sensors and Electron Devices Directorate (ARL-SEDD), and also 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 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 FY14, 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 FY14 were \$21.6 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY14 ARO Core (BH57) program funding allotment for this Division was \$5.6 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 \$9.6 million to projects managed by the Division. The Division also managed \$1.5 million of Defense Advanced Research Projects Agency (DARPA) programs, \$1.3 million for Minerva Research Initiative projects, and \$0.2 million was provided by other Army Laboratories. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided \$2.1 million for contracts. Finally, \$1.3 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes \$0.2 million of 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 FY14 (*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 FY14 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 FY14, the Division awarded 29 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to investigate optimal control policies for a class of static and dynamic stochastic optimization problems that have large, usually vector valued state spaces, create new approaches for social copy detection and community detection in large scale network scenarios, discover new approaches for numerically preserving the array of balance laws for momentum, mass, angular momentum, energy, vorticity, enstrophy, and helicity, and to explore robustness and adaptability, as they affect such diverse situations as the functioning of biological systems, from gene networks to societies. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor David Anderson, University of Wisconsin - Madison; *Stochastic Models of Biochemical Reaction Systems*
- Professor Laura Balzano, University of Michigan - Ann Arbor; *Subspace Methods for Massive and Messy Data*
- Professor Yuri Bazilevs, University of California - San Diego; *Fluid-Structure Interaction Simulation of Gas Turbine Engines Using Isogeometric Analysis*
- Professor Amarjit Budhiraja, University of North Carolina - Chapel Hill; *Theory and Applications of Weakly Interacting Markov Processes*
- Professor Wei Cai, University of North Carolina - Charlotte; *Numerical Methods for Studying Optical Absorption of Random Media and Quantum Dots for Solar Cell Designs*
- Professor Mung Chiang, Princeton University; *Social Learning Networks: From Data Analytics to Active Sensing*
- Professor Peter Chung, University of Maryland - College Park; *Techniques for Phonon Superposition Modeling of Shocks and Waves in Solids*
- Professor Tyrone Duncan, University of Kansas; *Studies in the Control of Stochastic Systems*
- Professor Michael Fiddy, University of North Carolina - Charlotte; *Development of Inverse Scattering-Structure Synthesis Methods: Subwavelength Scale Imaging-Metamaterial Design*
- Professor Daniel Forger, University of Michigan - Ann Arbor; *Modeling Subconscious Vision*

- Professor John Fricks, Pennsylvania State University; *Forward and Inverse Methods for Stochastic Models of Diffusing Particles in Complex Biofluids*
- Professor George Karniadakis, Brown University; *Numerical Methods for Propagating Uncertainty Across Scales and for Hybrid Stochastic-Deterministic Systems*
- Professor Nancy Kopell, Boston University; *Prefrontal Brain Rhythms and Rule-based Action*
- Professor Reinhard Laubenbacher, University of Connecticut; *Canalization: A Fundamental Design Principle of Gene Regulatory Networks*
- Professor Chihoon Lee, Colorado State University - Ft. Collins; *Probabilistic and Statistical Analysis of Complex Stochastic Networks*
- Professor Simon Levin, Princeton University; *Robustness and Adaptability in Complex Biological Systems*
- Professor Xiaolin Li, SUNY at Stony Brook University; *Robust and High Order Computational Method for Parachute and Air Delivery and MAV System*
- Professor Wei Ji Ma, New York University; *Measuring and Modeling Attentional Limitations in Split-Second Visual Decisions*
- Professor Scott McKinley, University of Florida - Gainesville; *The Stochastics of Movement Ecology*
- Professor Cass Miller, University of North Carolina - Chapel Hill; *Thermodynamically Constrained Averaging Theory for Multiscale Systems*
- Professor Assad Oberai, Rensselaer Polytechnic Institute; *Multiscale Methods for the Reliable Simulation of Multiphase Processes*
- Professor Leo Rebholz, Clemson University; *Long-term Stable Conservative Multiscale Methods for Vortex Flows*
- Professor Sheldon Ross, University of Southern California; *Stochastic Optimization Problems with Large State Spaces*
- Professor Paolo Rosso, Universitat Politècnica De València; *New Method for Social Copy Detection in Large-scale Scenarios*
- Professor Guglielmo Scovazzi, Duke University; *Continuous/Discontinuous Variational Multiscale Methods for Variable Density Flows*
- Professor Sunder Sethuraman, University of Arizona; *Scaling Limits in Stochastic Interacting Systems*
- Professor Alexander Tartakovsky, University of Connecticut - Storrs; *General Multidecision Theory: Hypothesis Testing and Changepoint Detection-Classification*
- Professor Byron Wallace, University of Texas at Austin; *Sociolinguistically Informed Natural Language Processing: Automating Irony Detection*
- Professor Chien-Fu Jeff Wu, Georgia Tech; *Binary and Hybrid Response Data in Sensitivity Testing: Sequential and Bayesian Optimal Designs*

2. Short Term Innovative Research (STIR) Program. In FY14, the Division awarded 10 new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to create predictive Bayesian kernel models based on sparse historical evidence of previous events, create a novel approach to solve inverse problems for a class of mechanistic models arising from systems biology, define an axiomatic framework as a basis for generating rigorous social models, and to model a PDE as a computational object from initial-boundary value problems. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Kash Barker, University of Oklahoma; *Sparse Event Modeling with Hierarchical Bayesian Kernel Methods*
- Professor Suzanne Bell, West Virginia University; *Bayesian and Non-parametric Statistics: Integration of Neural Networks with Bayesian Networks for Data Fusion and Predictive Modeling*
- Professor Robert Clewley, Georgia State University; *Surrogate Testing Methods for Exploratory Data-driven Modeling*
- Professor Jin-Oh Hahn, University of Maryland - College Park; *Solving Inverse Problems for Mechanistic Systems Biology Models with Unknown Inputs*

- Professor Robert Kirby, Baylor University; *Computer-aided Transformation of PDE Models: Languages, Representations, and a Calculus of Operations*
- Professor Jingchen Liu, Columbia University; *Rare-event Analysis and Computational Methods for Stochastic Systems Driven by Random Fields*
- Professor Guodong Pang, Pennsylvania State University; *Gaussian Random Fields Methods for Stochastic Fork-Join Networks with Synchronization Constraints*
- Professor David Sallach, University of Chicago; *Homotopy Types and Social Theory: Theoretical Foundations of Strategic Dynamics*
- Professor Zsolt Talata, University of Kansas; *Statistical Inference on Memory Structure of Processes and Its Applications to Information Theory*
- Professor Guo-Cheng Yuan, Dana-Farber Cancer Institute, Inc.; *Single Cell Analysis of Dedifferentiation and Transdifferentiation in Mammalian Regeneration*

3. Young Investigator Program (YIP).

No new starts were initiated in FY14.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY14 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Third Conference on Systems Approaches in Immunology and Infectious Diseases*; Santa Fe, NM; 10-11 January 2014
- *2014 Social Computing, Behavioral-Cultural Modeling, and Prediction Conference*; Washington, DC; 2-4 April 2014
- *Advances in Symbolic Computations: Emerging Methodologies and Applications of Computer Algebra*; Durham, NC; 26 April 2014
- *Modern Perspectives in Applied Mathematics: Theory and Numerics of PDEs*; Bethesda, MD; 28 April – 2 May 2014
- *Mathematical and Computational Aspects of Multiscale Materials Modeling Workshop*; Troy, NY; 10-11 June
- *Isaac Newton Institute Research Program Workshop on Interdisciplinary Approaches to Understanding Microbial Communities*; Cambridge, U.K.; 10-12 September 2014

5. Special Programs. In FY14, 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 one new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grant 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. Designing and Prescribing an Efficient Natural-like Language for Bots. This MURI began in FY07 and was awarded to a team led by Professor Mitch Marcus at the University of Pennsylvania. The goal of this project is to develop theory that will eventually enable bots to both understand and to be understood by humans, ultimately enabling functional human-bot teams.

Fluent and effective communication between warfighters is imperative to convey orders and intent and to ensure adequate situational awareness. All unit members must continually exchange information as the environment changes. As autonomous bots move onto the battlefield, they will also need to participate in these complex linguistic interactions. This almost necessarily means equipping them with natural language capabilities. The Soldier whose native language is English can communicate a rich range of information and intentions in English with little appreciable increase in cognitive load, even when the Soldier is under high stress. Soldiers cannot compromise these abilities for the sake of the bots; therefore, this research strives to bring the bots to the level of the Soldier. This research effort is organized in nine synergistic areas: Machine Learning & Stochastic Optimization, Human–Robot Interaction, Syntactic Analysis, Semantic Interpretation, Pragmatic Enrichment, Parameterized Action Representation, Formulating Specification for Robot Motion Planning, Corpus Collection, and Testbeds and Integrated Demonstrations.

In FY14, the team completed an additional year of work, funded by ARL-CISD to pursue questions and objectives within their realm of particular interest that had become approachable during the course of the investigation. In this additional period of performance, the team investigated the performance of new NLP theory involving parsing, linear temporal logic, parameterized action representations, and semantic structures involving joint inferencing in actual human-robot interaction. Work included conducting a workshop at ARL's Adelphi Laboratory Complex on Linear Temporal Logic (LTL), covering basic construction of LTL and how to add new verbs via LTL, through senior associate interactive work with ARL scientists, and through proof of principle experiments conducted by team personnel at ARL Adelphi involving LTL and the LTLMoP. They also conducted experiments in the feasibility of these new methods in actual robot systems such as Lego Mindstorm and the ARL PackBot. This work experimentally validated the theory developed in the MURI, and provided guidance for future efforts, all within environments utilized by the computational linguistics lab at ARL-CISD.

2. Analysis and Design of Complex Multi-scale Networks. This MURI began in FY08 and was awarded to a team led by Professor Jean Walrand of University of California - Berkeley. The goal of this research is to invent new mathematical theories and techniques that will enable modeling, analysis and control of complex multi-scale networks. These theories will ultimately enable the development of a unified framework for understanding and exploiting complex behaviors of the network resulting from spatial and temporal heterogeneity and the interaction of network algorithms with traffic characteristics.

More specifically, the objective of this MURI is to: (i) understand the interaction of traffic statistics, including long-range dependence (LRD) properties, and control actions across timescales, from back-clocking and burstiness effects at the sub-round-trip-time (sub-RTT) timescale, congestion control at RTT timescales, inter-domain routing at the time scale of minutes or hours, to revenue maximization and peering structure on the scale of days and months, (ii) design strategies for controlling admissions of new connections, flows of admitted connections, and the pricing of connections taking into account the LRD property of the traffic, (iii) develop theories for maximizing network utilization in the presence of wired and wireless links (which typically pose significant challenges for the proper utilization of network resources by end-to-end rate control protocols), and (iv) design traffic-measurement techniques in a heterogeneous environment, which can have significant implications for monitoring, management, and security of the network. The new distributed algorithms for wireless networks that may result from this work have the potential of revolutionizing *ad hoc* networks by enabling the design of simple, robust, and efficient protocols. Improved WiFi protocols increase the throughput by a significant factor and the fundamental theoretical research by this MURI team on LRD will produce new mitigation methods such as optimal fragmentation and diversity routing.

3. Discovering New Theories for Modeling and Analysis of Multi-scale Networks. This MURI began in FY08 and was awarded to a team led by Professor Ness Shroff at the Ohio State University. The objective of this research is to invent new mathematical theory and techniques in order to enable modeling, analysis and control of complex multi-scale networks. In particular, the research will develop a mathematical theory and techniques for modeling, analysis, and control of complex multi-scale networks.

The research team is investigating multi-scale phenomenon and control of wireless systems including LRD in wireless systems, which is a consequence of the temporal and spatial complexity inherent in military networks. The research focuses on the impact of multi-scale phenomena on the control, performance, and security of these networks. This research will lead to a long-overdue union of stochastic control, statistics, queuing theory, complexity theory, and the distributed algorithms, which is necessary for the development of radically new strategies for controlling the increasingly complex military networks.

The research approach consists of three inter-related focus areas: (i) traffic modeling and analysis, (ii) network control, and (iii) information assurance. While the investigation covers both wired and wireless networks, it focuses heavily on the wireless portion of the overall networks, which is central to tactical communications and the Army's network centric operations, and is likely to have the most stringent resource constraints and greatest vulnerability to security breaches. The modeling approach takes into account the critical time scales in military networks, from user-level applications (*e.g.*, time-critical data), to the time-scale required for the operations of various protocols and resource allocation schemes; this is significantly different from the state-of-the-art in traffic modeling, where the network is viewed as a physical entity whose laws are being passively observed through traffic studies. The team is formulating optimization and distributed control problems for providing network services and studies the impact of LRD traffic on network control, performance, and security. The project is also developing an integrative approach that combines the LRD modeling and network control to obtain non-parametric or semi-parametric techniques for the distributed detection of information flow and flow changes needed for preventing security attacks. The research is characterizing the ability of flow to be detected as a function of flow rate, delay and memory constraints, and develops distributed detection schemes that guarantee vanishingly low detection error probabilities. The outcomes of this project will result in distributed, low-complexity, and robust control mechanisms for achieving high network performance, intrusion detection, and security. These outcomes will provide high performance, reliability, and information assurance in support of the Army's future Network-Centric Operations and Network Centric Warfare (NCW). Further, the rigorous and conceptually unifying mathematical techniques developed in the course of this work will enable a deeper understanding of the dynamics and control of large and complex networks.

4. Network-based Hard/soft Information Fusion. This MURI began in FY09 and was awarded to a team led by Professor Rakesh Nagi of the University at Buffalo. The goals of this research are to develop a generalized framework, mathematical techniques, and test and evaluation methods for fusion of hard and soft information in a distributed (networked) Level 1 and Level 2 data fusion environment.

During the first four years of this effort, the MURI team developed and refined the overall system concept for human-centered information fusion and information processing architecture and developed an evolutionary test and evaluation approach that proceeds from "truthed" synthetic hard and soft data to human-in-the-loop campus based experiments. The researchers created, refined and analyzed a counter-insurgency (COIN) inspired synthetic data set ("SYNCOIN") involving both hard and soft data. The MURI team completed human-in-the-loop data collection activities involving hard sensors. The team developed a software package "Tractor" for processing text messages in multiple stages and common referencing; evaluated syntactic and semantic processing techniques and selected GATE (General Architecture for Text Engineering) for syntactic processing and FrameNet for a semantic processing database. The MURI team refined a soft data association prototype that extends the traditional hypothesis generation-hypothesis evaluation-hypothesis selection paradigm for fusion of soft data and utilizes a data graph association process.

During the fifth year, the MURI team made several notable accomplishments. The first known Hard and Soft "SYNCOIN" dataset for fusion technology and analytics development was finalized and distributed to ARL-CISD and to CERDEC. This counter insurgency dataset has about 600 natural language messages with interleaved vignettes for the development and testing of natural language processing methods, and hard sensor associable counterparts for developing semantic extraction and association technologies. This unique data sets is inspired by a Counter-Insurgency (COIN) scenario in Bagdad and contains synthetic soft (human report) data, synthetic hard (physical sensor) data, and real hard data collected using human-in-the-loop vignettes collected at a special facility in central Pennsylvania. The data are augmented by extensive "ground truth" information including, scene setter descriptions, identification and location of all events and activities, social network information, database schema, reference maps, and word cloud diagrams. The first-ever comprehensive characterization of human observations that are context sensitive was completed. Results have been submitted to the journal *Information Fusion***,** and transition to ARL-CISD is pending through the ARL infrastructure initiative. Characterizing the human observer has been determined to be an essential "human" source characterization and common referencing step for hard-soft fusion. A novel approach to Natural Language Processing through the software "Tractor", and context overlay has been accomplished so that no information is lost and all semantically meaningful information is extracted. Relevant contextual information (as a human would have when reading text) is added so that machine reasoning is feasible. This is a goal, but it is an important discriminator from NLP engines that are simply interested in "information retrieval" of entities and relationships. A best-in-class graph association engine has been developed, along with the first Map-Reduce implementation for distributed computing. The event association engine, which includes location normalization, has been competitively compared to others in the literature. These are described in a paper for Association for Computing Machinery (ACM) Transactions on Information Systems. Association results provide better precision, recall and F-measure than other approaches in the literature. Results have been published Parallel Computing and Naval Research Logistics and others. Hard sensor processing techniques and a system for processing text messages are in the process of transitioning to ARL-CISD and ARL-SEDD.

5. Mechanisms of Bacterial Spore Germination. This MURI began in FY09 and was awarded to a team led by Professor Peter Setlow at the University of Connecticut Health Science Center. The objective of this research is to decipher the biological mechanisms that underlie heterogeneity of bacterial spore germination with an emphasis on the slow germinating population.

Most bacterial spores readily and quickly germinate after being exposed to appropriate growth conditions, a small percentage do not. Within the population, individual spores may germinate days, weeks, or even months, with serious implications. In food processing, the presence of slowly germinating spores results in a need for harsh processing conditions, such as high pressure and temperature, leading to a loss of food quality and appeal. Medically, delayed germination can result in disease appearance after antibiotic therapy has been discontinued. This research team is using a combination of "wet lab" experiments and computational modeling to understand the fundamental mechanisms of spore germination. This research may ultimately lead to strategies for preventing bacterial spore germination that could be used in food processing and medically-relevant therapeutic technologies, and for the enhancement of spore germination to be used in new methods of biofuel production.

6. 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 two 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.

In the fourth year of investigation, the MURI team has encoded society+network connections (e.g., adjacency matrix with elements $\neq 0$ if tie exists), has 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. The team has recently developed new network community models, comprised of new mathematical theory coupled with sound sociological interpretation. The team has quantified latent social foci which interpret latent variables and recover hidden structure, and has made progress in developing new algorithms and models for sub-network discovery; these efforts continue in the final year of work. The team is also exploiting network heterogeneity in novel ways by accounting for temporal and other forms of variability.

7. Structured Modeling for 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.

8. 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.

9. 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.

10. 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.

11. 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, the 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.

12. 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.

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

No new starts were initiated in FY14.

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 FY14, 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 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 FY14, the Division managed two new ARO (Core) HBCU/MI projects, and one new REP award, 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 PECASE winners for each calendar year are typically announced by the White House at the end of the fiscal year. However, the 2014 PECASE recipients had not yet been announced at the time this issue of ARO in Review was completed. 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 FY14, the Division managed four new DURIP projects, totaling $0.9 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Geometric Representation Integrated Dataspace (GRID) Program

The vision of the GRID program was to establish the theoretical foundations and pragmatic implications of a compressive representation format for high-resolution 3D data of all sensor modalities. The envisioned GRID format would have accurately encoded the 3D geometry and surface properties of objects at various spatial scales and would have provided efficient storage, application, and exchange throughout multiple industries. There have been numerous attempts, often independent and industry-specific, to efficiently capture 3D geometry and surface properties. This program proposed to unify disparate approaches in all three stages, namely, data format, encoding and rendering in automatic procedures. While there is strong interest in 3D land topography, this program also considers other areas such as manufacturing and biomedicine. The full GRID program was not funded by DARPA but, as part of the process for proposing the GRID program, the Mathematical Science Division identified and initiated three pilot projects that were supported via DARPA funding. Many of this program's goals are complementary to the research directions pursued by the Division's Dynamic Modeling of 3D Urban Terrain MURI.

I. DARPA Economics of Collective Value Program

The objective of this program is to develop a theoretical framework that describes the dynamics of economic agents, transactions and price behavior, using a correspondence to physical non-equilibrium systems. ARO collaborated with DARPA to develop this topic. ARO also manages this project as a step toward developing metrics which may also apply to more abstract areas such as social media: an area in which ARO has established a new research program. The framework provides a theoretical basis for the relationship of "value" and "price" as a scientific basis for economic systems. Price and value are in contrast to traditional theory, not synonymous. Traditional theories of value do not incorporate the complex dynamics of social systems. Value is determined by desire of an individual for a good, price is determined by collective agreements on transactions to transfer that good. The PI's new theoretical framework quantitatively reproduces the complex dynamics of economic agents and the resulting price behavior of commodity markets. The PI is mathematically modeling the mechanisms that underlie collective social behaviors, such as bandwagon effects, and has found evidence of their destabilizing force on the markets in the aftermath of the financial crisis (see FIGURE 1). The PI demonstrated how an unregulated economic activity, derived from the concept of a self-correcting stable economy, does not achieve market efficiency. This framework, introducing the perspective of complex systems into theories of price formation, provides a new scientific basis for economic systems.

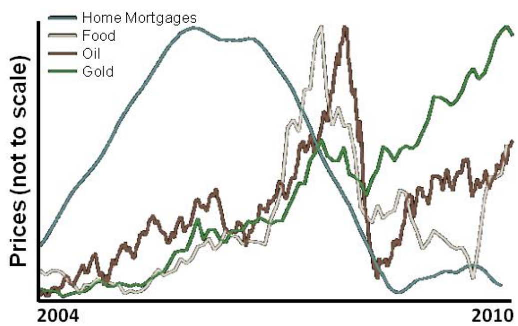

FIGURE 1

Historical commodity data. This commodity time series (2004-2010) plots relative changes in the prices of home mortgages (blue), food (yellow), oil (red), and gold (green), which are examples of the type of data used to text and validate theories developed by the research program.

J. 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.

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. Fast, Automated, Photo-realistic, 3D Modeling

Professor Avideh Zakhor, University of California-Berkeley, Single Investigator Award

The objective this research is to create approaches for 3D geometry modeling, plane fitting for complex environments, texture mapping, visualization and rendering to further improve a fast, automated 3D modeling system that produces a photorealistic, high resolution, 3D graphics database for the interior of buildings. The PI has investigated methods and algorithms for automated, human operated, portable, 3D indoor navigation and modeling, and a means of achieving photo-realistic rendering of internal structure of multi-story buildings. The motivation to focus on a human operated, portable system rather than an autonomous robot stems from speed, robustness, and scalability considerations, as well as the limitations of robots in complex environments such as stairways inside a building, uneven terrain, and dynamic environments. In addition, a human operator can ensure much more thorough data acquisition for all objects, surfaces, details, and furniture inside a building, than a robot could ever do. In the context of military applications, one can envision a group of soldiers capturing the necessary data to build interior or exterior 3D models while inspecting a multi-story building, or patrolling around a campus filled with buildings.

There are several unique and important questions involved in such an investigation. First, unlike a wheeled robotics system which exhibits only three degrees of freedom, namely x, y, and yaw, a human operator exhibits six degrees of freedom: x, y, z, yaw, pitch and roll. Even though it can be argued that pitch, roll and z are small for typical human gait, they cannot be ignored during the localization and model construction process. In addition, since this involves modeling complex environments such as staircases, wheel odometry measurements typically used in robotics systems cannot be applied here. Also, lack of GPS inside buildings requires new ideas for localizing the acquisition system in indoor modeling applications. Finally, this must be done under severe weight and size constraints since it will ultimately be realized as a human operated system in which a person carries a backpack full of sensors and equipment. The major challenges for such a modeling algorithm can be summarized as follows:

- System architecture: What sensor components should be used? What is the spatial, or geometric configuration of the sensors? How many sensors are sufficient to fully capture geometry and texture?
- Localization algorithms: How should the data from heterogeneous sensors be combined to accurately localize the backpack? Localization here means recovery of pose, i.e. x,y,z, yaw, pitch and roll. Without localization, it is not possible to generate a 3D point cloud made of the laser scan returns.
- Geometry modeling: Once localization is completed and a 3D point cloud is generated, what is the best way to model the environment? Traditionally, triangulation has been applied to 3D point clouds to result in meshes. However, planar approximation of walls and floors could potentially result in better looking, more artifact free models, even though they could oversimplify the environment or could fail in complex structures such as staircases.
- Texture mapping: Given that the texture for each piece of geometry in a model is captured by multiple cameras, and by multiple frames in a given camera, how is texture selection to be accomplished? Lack of neighborhood consistency can result in disturbing visual artifacts.
- Visualization and rendering: What is the best way to interact with the resulting models? The size of resulting models is generally too large to be viewed with today's renders without Level of Detail (LoD) simplification. Yet LoD simplification needs to be applied in such a way so as to avoid disturbing visual artifacts at the boundaries. Can image based rendering be used to visualize the scene without explicitly constructing a 3D model? When revisiting the same location during the walkthrough, one can enforce a "loop closure" since the loop has been closed by revisiting. Any deadreckoning algorithm has errors that accumulate over time since they are incremental. So, when revisiting the same location, the deadreckoning algorithm output does not always detect or indicate that one is in the same place.

In FY14, the PI developed and implemented Rao-Blackwell-Particle Filtering and related methods to determine if/when one has revisited the same spot. Once that has been detected, then a constraint is enforced to define this spot as being close to another spot that was visited some time ago. This "closes the loop," and allows a graph optimization problem to be solved to refine the locations at all times, even before the revisit (see FIGURE 2). Successive scans are matched from the X-Y scanner in an attempt to determine the 2D change in position and orientation i.e. to obtain delta-x, delta-y and the angle change in the x-y plane. It turns out that when matching temporally successive scans, the initial condition of one pair is the final answer of the previous (temporally) pair. However, when revisiting the same location after some time later, doing scan matching between those two becomes ill-conditioned since there is no longer a good initial condition. Therefore it has been found optimal to do scan matching both across successive scans and also when the scans are not successive (i.e., after traveling some period of time to revisit the same location). It has been found that deriving positions by integrating accelerometer data is too noisy; therefore using an x-y scanner and scan matching to derive position and yaw orientation is found to be optimal. Vetting is conducted after estimating the transformation at a loop closure in order to determine whether that transformation is good or bad. If it is bad and was to be used in the graph optimization algorithm, it is found to introduce significant errors in path recovery and the resulting point clouds. So, it is found that tossing out loop closures which cannot be vetted properly is expensive but most effective. This method transitioned to ARL-CISD in the form of a complete system, with algorithms loaded and has been discussed with CERDEC.

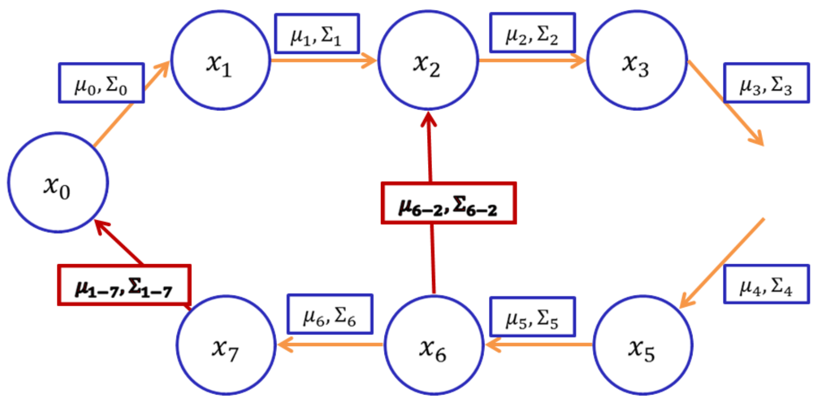

FIGURE 2

Position localization algorithm. This involves fusing dead reckoning and particle filtering with a graph optimization approach, extracting global constraints using those as loop closure constraints, and combining these via optimization in order to obtain a geometrically consistent, full data rate path.

B. Optimal Control of Stochastic Systems Driven by Fractional Brownian Motion

Professor Tyrone Duncan, University of Kansas, Single Investigator Award

The objective of this research is to solve stochastic control problems by obtaining explicit optimal controls for linear or nonlinear stochastic systems that are driven by fractional Brownian motions or more generally other stochastic processes with continuous sample paths and that have cost functionals that are quadratic in the state and the control. The solution of control problems for discrete time linear systems with quadratic cost functionals with arbitrary correlated noise is also an objective. These general noise processes both in continuous and discrete time are important in models for many physical phenomena (e.g. turbulence, cognition, telecommunications, and medicine).

In FY14, the PI and co-PI have developed methods to achieve explicit optimal controls by a direct method. The significance of this research is the construction of explicit optimal controls for a variety of basic models. In particular, explicit optimal controls for linear and nonlinear stochastic systems that are driven by Brownian motion, fractional Brownian motions or general processes and optimal control strategies for two player linear and nonlinear stochastic differential games with Brownian motion or general noise processes have been obtained. From the explicit optimal controls obtained in this research, applications of optimal control can be made to a variety of important physical systems. These results allow for the physical implementation of optimal controllers for such problems as turbulence and telecommunications.

C. Nutrient-cycling Microbial Ecosystems: Assembly, Function and Targeted Design

Professor Rosalind Allen, University of Edinburgh, Single Investigator Award

Despite a wealth of new information emerging from DNA sequencing technologies, our basic understanding of the principles underlying the structure and function of microbial communities involved in bioremediation remains very poor. The objective of this research is to reveal fundamental principles underlying the assembly and function of nutrient-cycling microbial communities, using a combination of mathematical modeling and laboratory experiments. The specific aims are to (i) understand the assembly dynamics of a microbial nutrient-cycling ecosystem, (ii) investigate its response to environmental change, and (iii) apply these principles to the targeted design of microbial communities for applications in bioremediation. To achieve these aims, this research combines theoretical and experimental work. On the theoretical side, the models are based on ordinary differential equations, in which variables represent the population densities of different microbial metabolic types, and the concentrations of key chemical species. The growth of a given population depends on the concentration of its food sources, and as it grows it excretes waste products that can be used as food by other populations. In FY14, the models have assumed "well-mixed" populations; models with greater spatial resolution are beginning to be developed. On the experimental side, laboratory microcosms, made from pond sediment and water, and supplemented by carbon and sulfur sources, are used. Over several months these microcosms develop into vertically stratified, stable, nutrient-cycling communities which allow tracking of the development of chemical gradients using voltammetry and microbial community composition by extraction, fingerprinting and sequencing of DNA.

In FY14, the community and chemical composition of nutrient-cycling communities were characterized experimentally as they assemble, and '2-box' models (see FIGURE 3) were developed for the microbial population dynamics. Significantly, a peak in sulfide was observed in all of the mesocosms at a time and height dependent on the amount of carbon source added (see FIGURE 4). Because sulfide is toxic, this finding implies severe consequences of organic matter pollution in nutrient-cycling ecosystems. Progress was also made in theoretically analyzing responses to perturbations and experimentally studying the effects of cellulose addition. This work demonstrated that changes in organic matter or oxygen availability can trigger redox 'regime shifts' (see FIGURE 3) and suggests an urgent need for better description of microbial population dynamics in biogeochemical models.

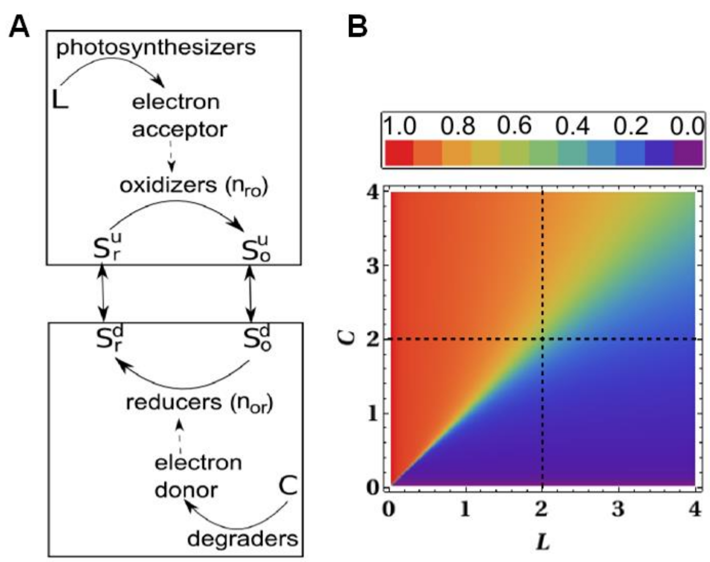

FIGURE 3

The "four-population, two-box" mathematical model and its predictions for redox regime shifts. (**A**) Illustration of the model. Oxidative and reductive processes take place in separate spatial zones, linked by chemical diffusion. (**B**) Steady-state fraction of sulfide as a function of the light intensity (L) and concentration of organic carbon, C. The system shows a sharp transition in its oxidation level as the environmental parameters are varied.

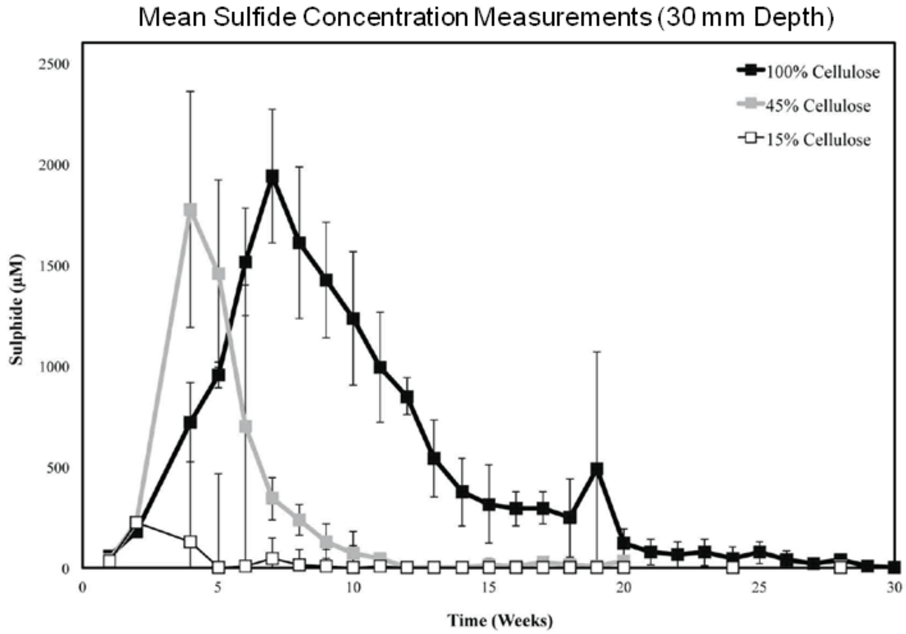

FIGURE 4

Results of the dynamical tracking of microcosm development. The concentration of sulfide within the sediment layer is shown as a function of time for microcosms with different added amounts of cellulose. Each dataset is averaged over multiple microcosms, with the error bars showing standard deviation. The data shows a distinctive peak in the sulfide concentration at a time that depends on the amount of cellulose added. Interestingly, a second peak is also observed. A key objective for the mathematical model in FY15 will be to explain this data.

D. Globally Convergent Methods for Coefficient Inverse Problems

Professor Michael Klibanov, University of North Carolina - Charlotte, Single Investigator Award

The objective of this research is to develop a globally convergent numerical method for coefficient inverse problems. In FY14, noteworthy accomplishments were completed in the mathematical theory of the global convergence, in the computation of unknown coefficients using this theory, and in numerical testing in a scenario of Army interest. The main drawback of the conventional method, involving minimization problems involving Tikhonov functional, is that it is non-convex. Thus, as a rule, it has multiple local minima and ravines. This, in turn causes local convergence of numerical methods of minimizations of such functionals, such as, e.g. gradient method and Newton method. The local convergence is a serious deficiency of those numerical methods for Coefficient Inverse Problems since convergence of such a method is guaranteed only if its starting point is located in a sufficiently small neighborhood of the solution. However, a reliable knowledge of that neighborhood is rarely available in applications. The fundamentally new feature of this method, distinguishing it from all others, is the rigorous guarantee of obtaining a good approximation for the unknown coefficient without any advance knowledge of a good first guess. The main new element of this functional is the presence of the Carleman Weight Function (CWF), i.e. the weight function, which is involved in the Carleman estimate for the underlying hyperbolic operator. The main new result is a theorem which guarantees that, given a certain convex set G of an arbitrary finite size in a Hilbert space, one can choose the large parameter of this CWF in such a way that the above weighted Tikhonov-like functional is strongly convex on this set. Appropriate definition of the set G is made. Since restrictions on the size of G are not imposed, this is termed global strong convexity. Thus, the property of the global strong convexity manifests the fundamental difference between weighted Tikhonov-like functional and the conventional Tikhonov functional. Indeed, the latter one is non-convex, which, unlike this case, causes the above mentioned phenomenon of its multiple local minima and ravines (see FIGURE 5A). The PI has proven that initial iterants are guaranteed to contract toward a global solution. Research conducted by the PI established the result theoretically, and has been implemented on experimental data, including the case of blind data for objects buried in sand (see FIGURE 5B and FIGURE 6).

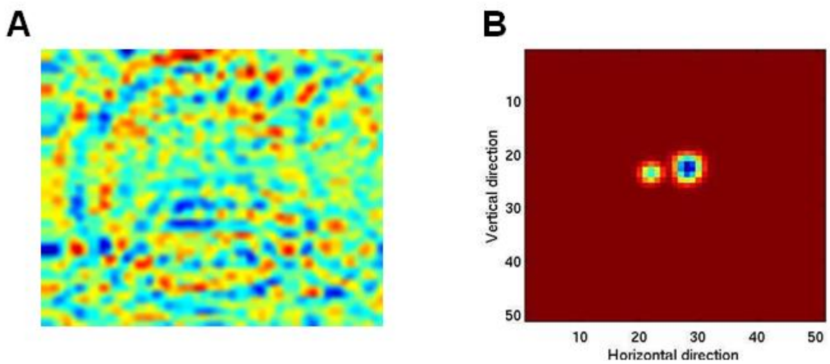

FIGURE 5

Laplace transforms of the data on the propagated plane. Results are shown (A) before the extraction of the targets' signals, and (B) after the extraction of the targets' signals. After extraction, two targets show up clearly.

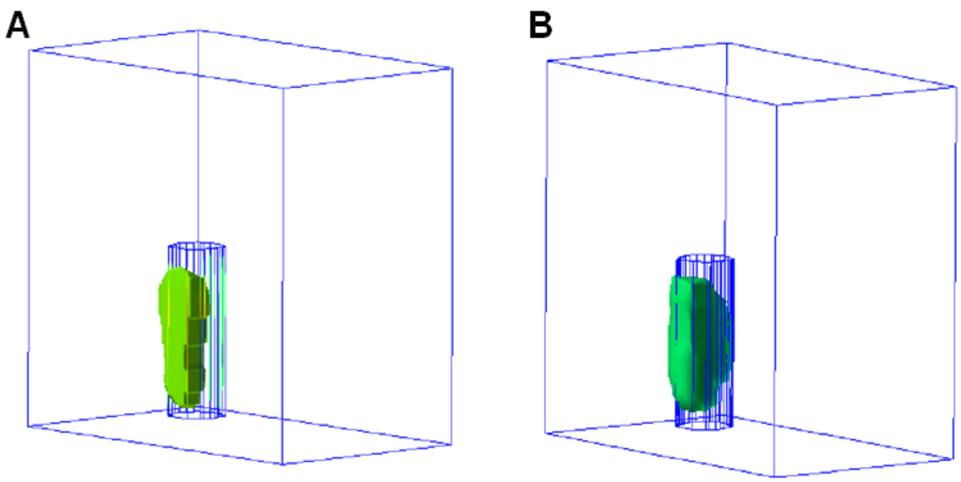

FIGURE 6

Reconstruction of a plastic bottle filled with clean water. Results are shown from (A) globally convergent method (stage 1), and (B) with adaptivity.

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 to external organizations and customers.

A. Structured and Collaborative Geometrics Signal Models for Big Data Analysis

Investigator: Professor Guillermo Sapiro, Duke University, Single Investigator Award
Recipient: National Geospatial Agency

Efficient data modeling is critical for ill-posed problems in signal reconstruction, classification, and identification. The objective of this research is to create a fundamental framework for structured and collaborative design of such signal models. The underlying foundations are derived via a combination of theories from sparse modeling, Gaussian Mixture Models, and Principal Component Analysis. Efficient computational approaches have been considered and developed as well. In addition to theoretical and computational questions, particular applications include anomaly detection in videos with a dynamic background, collaborative object detection and classification, source identification and separation, activity clustering in video, and dimensionality reduction onto physical meaningful spaces. The combination of multimodalities and incorporation of prior knowledge and side information is also considered. Scenarios with significantly undersampled or missing data have also been addressed in this framework. The theoretical foundations include the development of a novel approach of collaborative compressed sensing and the incorporation of information theory tools into the sparse modeling world. In order to address critical big data challenges, on-line and real time optimization techniques have also been developed.

Many have used Gaussian Mixture Models (GMMs), but dropped these, deemed them not powerful enough for image processing. This started to change with the PI's 2012 paper which clearly demonstrated that when properly done, GMMs are very powerful. The PI properly solved the GMM estimation for the first time with smart initial conditions (learned from years of literature on sparse modeling), stable covariance estimation, and very computationally efficient methods. After that, and after being complemented by good theoretical foundations in other related work in statistical compressed sensing of GMMs, the PI applied it to other challenges, such as the construction of adaptive sensing matrices and video cameras. Such a camera was the result of great team collaboration, merging a variety of unique expertise. The result was the first connection of GMM's with structured and collaborative sparse modeling, which inherited the benefits of both theories.

The key insight for doing sparse modeling in real time is not to continue the use of variations in optimization techniques, where most efforts have been concentrated, but to realize that sparse modeling can be considered as a map from the signal to the code, and what is needed is to learn the map. Then, combining the progress in sparse coding with activities in neural networks, the PI proceeded to learn that map (i.e., function), where the optimization techniques dictated the basic architecture of the network. This has turned out to be a very novel way to look at optimization. The most important mathematical contributions are: (i) in GMM, the PI showed bounds on the number of samples needed to reconstruct the model, showing that the bounds are more favorable than those when the model follows simple sparsity (as in standard compressed sensing), and then extended and combined this with Bayesian modeling and adaptive sampling to lead to the sensing paradigms developed; (ii) in the work on the representatives, they explicitly proved that the representatives are the vertices of the convex hull for each one of the subspaces present in the data (giving also a new way to compute convex hull in high dimensions) and also how and when representatives can be used to cluster data; (iii) related to learning, the PI formally proved where multimodal labels are useful and where they are not, the first result that does a comprehensive analysis of the value of multimodal labels in supervised learning scenarios; and (iv) in the optimization work, the PI opened a whole new area of theoretical questions deriving from this new perspective to optimization, such as in symmetry detection (see FIGURE 7).

This work was coordinated with and followed by the National Geospatial Agency (NGA). NGA designated the technology from this project as their Transition of the Year, and has hired Dr. Castrodad, the student who did his thesis work on this research.

FIGURE 7
Symmetry detection automated through Gaussian Mixture Models.

B. Modeling, Analysis, and Algorithms for Stochastic Control of Multi-Scale Military Networks
Investigator: Professor Ness Shroff, Ohio State University, MURI Award
Recipient: Communications-Electronics Research, Development and Engineering Center (CERDEC) and ARL-Computational and Information Sciences Directorate (ARL-CISD)

The objective of this research is to create the theoretical foundations for modeling, analysis, and control of multi-scale military networks to achieve high network performance. In FY14, the team made significant progress towards this goal. In particular, they developed an understanding of the causes of multi-scale phenomenon including long-range dependence (LRD) in wireless systems and how to model them in the presence of fading channels and spatial-temporal correlations. They have made significant progress in their investigation of the impact of wireless network protocols on traffic characteristics, in terms of traffic burstiness, self-similarity and long range dependence. They have developed tools for controlling multi-scale network traffic that go beyond the traditional realms of throughput maximization and stability, and have begun to uncover the impact of delay on such systems. The team has investigated the impact of LRD traffic on network control with focus on multi-scale decompositions. The team has also developed a unifying framework for designing low-complexity scheduling policies in the downlink of multi-channel (e.g., OFDM-based) wireless networks that can provide optimal performance in terms of both throughput and delay. Finally, they have developed traffic models that incorporate timing information in network systems for inference and information assurance. Based on the characterization of flow detectability, they have designed low-complexity detection systems for security attacks, user behaviors, and social connectivity, and investigated the development of distributed systems with local information.

The research team has collaborated with CERDEC scientists and engineers on modeling-simulation-validation of mobile adhoc networks through a Phase II SBIR with the company AIMS, Inc. The collaboration also included transferring modeling and simulation software which is being used by CERDEC to simulate the traffic flow in mobile adhoc networks, and joint investigation into causes of LRD and heavy tails in MANET based on the mobility patterns has been performed by CERDEC. The models and performance of MAC protocols produced by the MURI team members have been transferred to CERDEC who is using the scheduling based MAC protocols for MANET to detect the presence of LRD and heavy tail traffic. The research team has also collaborated with ARL scientists and engineers on studying the implications of traffic stochastic models of mobile wireless networks on network security and information assurance. The algorithms produced are being used by ARL-CISD in detecting wormhole attacks.

C. Mechanisms of Bacterial Spore Germination and its Heterogeneity
Investigator: Professor Peter Setlow, University of Connecticut, MURI Award
Recipient: Natick Soldier Center (NSRDEC)

The objective of this research is to gain a detailed understanding of the germination of spores of *Bacillus* bacteria, particularly to understand the reasons for heterogeneity in germination of spores that are extremely slow to germinate, termed superdormant (SD) spores (see FIGURE 8). Dormant spores of *Bacillus* and *Clostridium* species are major agents of food spoilage and food borne disease and spores of *B. anthracis* are a major potential biowarfare agent. Thus there is great interest in the DOD in methods to inactivate spores or otherwise prevent their "return to life" in germination. The fact that germinated spores are much easier to kill than dormant spores is another reason for the DOD's interest in spore germination, in particular into the causes of the extreme heterogeneity in spore germination that give rise to so-called "superdormant" spores that only germinate extremely slowly. Spores of *Bacillus* species can remain in their dormant and resistant states for years, but exposure to agents such as specific nutrients can cause spores' return to life within minutes in the process of germination.

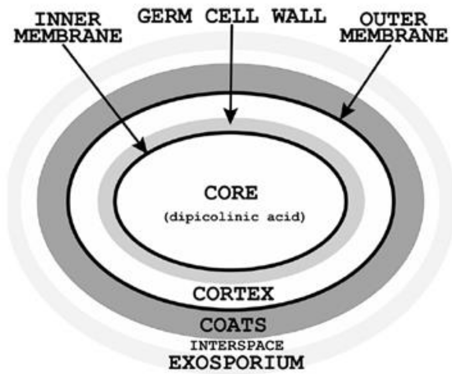

FIGURE 8

Outline of the structure of a *Bacillus* spore. The sizes of the various spore layers are not drawn to scale, spores of some species lack an exosporium, and at least for *B. subtilis* spores, there are several coat layers, as well as a layer outside the coats termed the "crust." All spore dipicolinic acid is in the spore core. Note that a defining feature of spores that have an exosporium is the layer between the coat and exosporium designated the interspace, although the precise composition of this interspace layer is not known.

By its fifth year of MURI support, this project has made significant progress in understanding how this process occurs (see FIGURE 9), discovering that this process requires a number of spore-specific proteins, most of which are in or associated with the inner spore membrane (IM). These proteins include the (i) germinant receptors (GRs) that respond to nutrient germinants, (ii) GerD protein, which is essential for GR-dependent germination, (iii) SpoVA proteins that form a channel in spores' IM through which the spore core's huge depot of dipicolinic acid is released during germination, and (iv) cortex-lytic enzymes (CLEs) that degrade the large peptidoglycan cortex layer, allowing the spore core to take up much water and swell, thus completing spore germination.

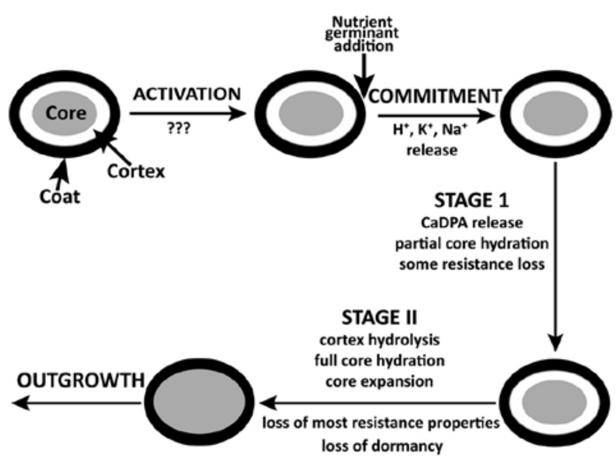

FIGURE 9

Schematic outline of nutrient germination of spores of *Bacillus* species. The precise events in the activation step are not known and are therefore denoted as question marks. The first step seen following the addition of a nutrient germinant to an activated spore is commitment, and the release of monovalent cations is associated with commitment. The germ cell wall is not shown in the figure, but this expands somehow as the cortex is hydrolyzed in stage II of germination.

In particular, mathematical modeling has been tightly coupled to experimentation in order to make this progress in understanding the mechanics of bacterial spore germination. The team has developed a mathematical model of bacterial spore germination that accounts for heterogeneity in time to commitment to germination and time to release of spore dipicolinic acid. The model is built from three main mathematical components: a receptor distribution function characterizing the probability of a given spore having a particular number of GRs, a receptor activation function that determines what fraction of a spore's GRs are active given a set of nutrient concentrations, and a germination kinetics function that specifies the number of active GRs a spore must contain in order to germinate by a given time t. This model is then used to predict the fraction of spores germinating as a function of time and germinant concentration.

Detailed knowledge of the mechanisms of spore germination and causes of superdormancy may lead to a new methodology for spore germination and thus easier spore eradication and decontamination, both of significant interest to the DoD for the purpose of preventing food spoilage. Due to this common interest, significant and ongoing collaboration has taken place between several of the labs involved in the MURI and Natick Soldier Center. This collaboration has resulted in two refereed publications in the past year, an additional paper in press, and ongoing work on the effects of heat activation on high pressure induced spore germination.

D. Parallel Sparse Linear System and Eigenvalue Problem Solvers for Multicore to Petascale Computing
Investigator: Professor Ahmed Sameh, Purdue University, Single Investigator Award
Recipient: ARL Weapons and Materials Research Directorate (ARL-WMRD)

The objective of this research is to investigate linear solvers and eigenvalue solvers in the context of new multicore architectures and bandwidth constraints imposed by potential speeds up to exaflops. Rapid advances in high-end computing architectures have posed new challenges in the design of algorithms that are capable of achieving significant parallel scalability, particularly for sparse matrix computations. This project has been investigating parallel scalable solvers for both large sparse linear systems, and for large sparse Hermitian generalized eigenvalue problems. The goal is to extend our understanding to achieve efficient performance on multicore architectures as well as scalability on petascale and future exascale architectures.

The algorithms that have been developed can be used either as direct solvers or as solvers of very effective “generalized banded" preconditioners of outer Krylov subspace schemes. One very effective developed scheme (TraceMIN) computes a few of the lowest eigenpairs of large, sparse real symmetric eigenvalue problems, as well as the Fiedler vector of the Laplacian associated with the sparse matrix graph for weighted spectral reordering; these can be used to help extract effective “generalized banded" preconditioners. Both classes of parallel algorithms appear to be of great effectiveness in a variety of computational science and engineering applications including structural mechanics, computational nano-electronics, and computational chemistry.

The PI's team collaborated with ARL-WMRD scientists in the latter stage of the project in order to verify and validate their algorithms and to measure performance increase. Inserting these algorithms into WMRD code demonstrates an order-of-magnitude cost savings in time required to perform large-scale quantum mechanical calculations. One significant component of the innovation is an intelligent sparse matrix reordering as a preprocessing stage that essentially avoids a huge number of unnecessary calculations. This is accomplished by permuting the equations to cluster the extraneous portions together, and then skipping those portions so that roughly 90% fewer calculations are performed. These techniques are also planned to be explored for use in joint work that is now beginning with ARDEC in simulation of multiscale/multiphase processing.

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. Semi-inner-products in Banach Spaces with Applications to Regularized Learning, Sampling, and Sparse Approximation

Professor Jun Zhang, University of Michigan, Single Investigator Award

The objective of this research is to fully develop Banach space methods for kernel-based machine learning that extend the Hilbert space framework of regularized learning. Specifically, the research will investigate Reproducing Kernel Banach Spaces (RKBS) by the semi-inner-product, develop the theory of vector-valued RKBS with applications of RKBS to manifold learning, study frames and Riesz bases for sequence spaces, and construct RKBS with the `1-norm known to enforce sparse solutions. The PI will seek to develop classification algorithms that are mathematically rigorous while rooted in human cognitive principles for categorization (generalization by similarity, feature selection by attention, etc).

It is anticipated that in FY15, the PI will take advantage of existing results in Hilbert space, and generalize them to a Banach space setting by replacing the inner product with the semi-inner-product. The semi-inner product behaves in a much similar way (and plays essentially the same role) as that of an inner product, except that many problems that are linear in the Hilbert space formulation become nonlinear. However, since the nonlinearity is of a special kind, involving the (generally nonlinear) duality mapping that is still one-to-one so long as the underlying Banach space is reflexive and strictly convex, therefore most Hilbert space results carry through to such Banach spaces. For non-reflexive Banach spaces (such as L1), the attempt will be to combine semi-inner-products with tools and techniques in sampling and approximation theory, reproducing kernel theory, frame theory, and measure theory to tackle the sparse learning problem.

B. Mutlivariate Heavy Tailed Statistics

Professor Sidney Resnick, Cornell University, MURI Award

The objectives of this research include generating new classes of multivariate heavy tailed models that account for implications of dependence and tail weight which can be calibrated to data, to develop reliable diagnostic, inferential and model validation tools for heavy tailed multivariate data, and to apply these statistical and mathematical developments to key application areas of social network analysis, network design and control, network security and anomaly detection, risk analysis, signal processing, and scheduling. Existing inference methods for heavy tail multivariate statistics are incomplete and subject to user interpretation about where to threshold and thus the inference methods are difficult to include in larger automated software routines that take the results of inference calculations as inputs. Existing methodology is typically for static, available, already collected data sets. New methods must automate the threshold selection and decide where the heavy tails begin; they will also fetch and process data in an on-line and real-time manner. Improved graphical tools aid model selection, confirmation, and exploration, and improved inference methods and software allow more sophisticated modeling with the potential for understanding cause and effect. Similarity testing will provide the capability of classifying large, dependent datasets exhibiting multivariate heavy tail statistics into “similarity classes.”

It is anticipated that in FY15, the MURI team will solve the thresholding problem using change point and goodness of fit methods and these methods will be automated by software. The team also aims to better understand model dependence between in-degree and out-degree of the social network models and will be able to determine how existing heavy-tailed diagnostics apply to network data and what further diagnostics for multivariate heavy-tailed distributions are applicable to social networks.

C. Prefrontal Brain Rhythms and Rule-based Action
Professor Nancy Kopell, Boston University, Single Investigator Award

The objective of this research is to understand how the dynamics of the brain affect how rules are carried out. Neural oscillations are associated with all facets of cognition; however, the way in which such brain dynamics support cognition is only beginning to be addressed. An understanding of how brain dynamics modulate and control learned rules that guide action can lead to a deeper understanding of the neural basis of higher cognitive activity. To address this question, computational models will be built that are constrained by in vivo and in vitro data and their properties investigated by simulation, leading to new ideas as to how the prefrontal cortex controls the execution of rule-based action.

It is anticipated that in FY15, the PI will focus on model building in close collaboration with experimentalists. All modeling will involve differential equations describing biophysical changes in cellular membrane potentials and will begin with a preliminary component model of the lateral prefrontal cortex, with network rhythms in the model constrained by physiological data on rhythms observed in isolated rat cortex. By the end of FY15, the component models will be refined and coupled, and simulations will begin testing task-related hypotheses.

D. Local-Global Model Reduction for Large-Scale Models Integrating Systems
Professor Eduardo Gildin, Texas A&M, Single Investigator Award

The objective of this research is to study reduced-order modeling methods for multiscale processes in heterogeneous subsurface formations. It is anticipated that in FY15, the PI will investigate a new local-global multiscale model reduction framework based on system theory and multiscale techniques for processes governed by complex systems. The concepts aim at reducing the degrees of freedom in the simulations by computing a mapping from input to output spaces, where the number of state variables and local multiscale basis are minimal. In addition, the PI will attempt to derive a priori error estimates which balance the error from global reduced-order models and local multiscale approximations. This effort involves two experienced interdisciplinary research groups from Texas A&M University and is unique in that it consolidates expertise in subsurface flow engineering and system and control theory with the formulation and analysis of multiscale methods in heterogeneous media. The understanding developed here has the chance to significantly advance the current state-of-the-art in multiscale model reductions and their applications to problems with multiple scales, parameters, and high contrast. These, in turn, will improve our ability to efficiently compute the solutions of large-scale systems that arise in the discretization of problems of linear and nonlinear flows in highly heterogeneous media.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Joseph Myers
Division Chief
Program Manager, Computational Mathematics

Dr. Harry Chang
Program Manager, Probability and Statistics

Dr. John Lavery
Program Manager, Modeling of Complex Systems

Dr. Virginia Pasour
Program Manager, Biomathematics

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 2014* is to provide information on the programs and basic research supported by ARO in fiscal year 2014 (FY14), and ARO's long-term vision for transitioning 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 FY14.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mechanical Sciences Division supports research to advance the Army and Nation's knowledge and understanding of the 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) advance knowledge and understanding governing the influence of inertial, thermal, electrical, magnetic, impact, damping, and aerodynamic forces on the dynamic response of complex systems as well as improving the inherent feature set of the components (*i.e.*, mechanisms and sensing) that comprise them, (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. In addition to advancing worldwide knowledge and understanding of properties and processes in mechanical sciences, 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 energy harvesting systems, 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 laboratory interactions of this Division are with the ARL Weapons and Materials Research Directorate (ARL-WMRD), ARL Vehicle Technology Directorate (ARL-VTD), ARL Sensors and Electron Devices Directorate (ARL-SEDD), the Joint IED Defeat Organization (JIEDDO), 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 also 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 FY14, 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 Area is to develop physically-based mechanics tools (theory, experiments, computation) for the quantitative prediction, control, and optimization of Army systems subjected to extreme battlefield environments. Army systems are frequently limited by material strength and failure. Solid mechanics research plays a crucial role in the prediction of strength, damage, and failure of Army materiel systems, structures and injuries of personnel under extreme loading conditions such as impact or blast as well as normal operating conditions. Research in computational and experimental solid mechanics forms the foundation of optimization tools to enhance performance while minimizing weight and volume, and its theories provide a strong link between the underlying physics of solids and the design of actual systems resulting in reduced development cost by minimizing the need for expensive system and field testing and it leads to novel ideas and concepts for revolutionary capabilities.

This Program Area is divided into two research Thrusts: (i) Multiscale Mechanics of Heterogeneous Solids, and (ii) Multiscale Mechanics of Biological Tissues. The goal of research in the Multiscale Mechanics of Heterogeneous Solids Thrust is to extend the design envelope of current and future Army structures for predictive continuum damage and cohesive models with a physical basis that is supported by computational modeling and experiments at the appropriate length and time scales. The objective of research in the Multiscale Mechanics of Biological Tissues Thrust is to understand how high rate loading of different durations and amplitudes may lead to cascading events starting at the cellular level that cause functional loss and impairment of human tissues and organs.

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 technology, including nanotubes, nanocrystaline 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, unmanned aerial vehicles (UAVs), unmanned ground vehicles (UGVs), and munitions.

2. Complex Dynamics and Systems. The goal of the Complex Dynamics and Systems Program Area is to develop new scientific understanding in three major research Thrusts: (i) High-dimensional Dynamical Systems, (ii) Force generation, Power and Work in Nonequilibrium Dynamical Systems, and (iii) Creating Quantitative Understanding of the Principles Underlying Biological Agility. 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, and (4) Control and Creation of Critical Dynamics.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). A common theme amongst all programmatic thrust areas is that systems of interest are "open" in the thermodynamic sense (or, similarly, dissipative dynamical systems). 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 ARL Major Laboratory Programs 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 kinetic models for heavy hydrocarbon fuels, novel kinetics model reduction methods, 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. The vast majority of the Army weapon systems involve airborne vehicles and missile systems that are totally immersed in fluids. In turn, the performance of these weapon systems is greatly affected by the resultant forces imparted on them by the surrounding fluid. Consequently, developing highly accurate, stable, agile, and long-endurance weapon systems dictates the need for fluid dynamics research in the areas of interest to both rotorcraft vehicles and tactical missiles. In fact, the battlefield capability and tactical flight operations envisioned for the highly mobile Army of the twenty-first century can only be accomplished through scientific breakthroughs in the field of aerodynamics. Improving performances in every aspects of rotorcraft vehicle performance requires intensive fluid dynamic research in areas, such as, unsteady boundary-layer separation on the suction side of rotorcraft blades, unsteady rotor aerodynamic loads, wakes and interference aerodynamics, and computational fluid mechanics.

Ongoing research topics within this Program Area include the experimental and numerical determination of the flowfield over airfoils undergoing unsteady separation with subsequent dynamic stall, the development of micro-active flow control techniques for rotor download alleviation and dynamic stall control, and the development of advanced rotor free-wake methods to improve the predictive capability for helicopter performance, vibration, and noise. To ensure the accuracy and range of unguided gun-launched projectiles and the maneuverability and lethality of guided missiles and rockets, a thorough knowledge of the forces and moments acting during both launch and free flight is required. These objectives dictate research on shock boundary-layer interactions, compressible turbulence modeling, aft body-plume interactions, vortex shedding at high angle of attack, transonic body flows, and aerodynamic interference effects between various missile components. Examples of current studies in this subfield are the experimental study of aft body-plume-induced separation, and the use of direct numerical simulation, laser-Doppler velocimetry (LDV), and PIV techniques to investigate axisymmetric supersonic power-on/power-off base flows. Research initiatives on the aerodynamics of small unmanned aerial vehicles, both rotary wing and flapping wing, continue. Results indicate that the physics of vortex-dominated flight at low Reynolds number is quite different than that encountered for familiar high Reynolds numbers.

C. Research Investment

The total funds managed by the ARO Mechanical Sciences Division for FY14 were $20.8 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY14 ARO Core (BH57) program funding allotment for this Division was $6.9 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 $3.8 million to projects managed by the Division. The Division also managed $7.8 million of Defense Advanced Research Projects Agency (DARPA) programs. Finally, $2.3 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.3 million of 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 FY14 (*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 FY14 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 FY14, the Division awarded 18 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to understand how high-amplitude, high frequency thermoacoustic emissions interact with turbulent shear layers associated with separated flows for potential flow control applications, discover/ quantitative principles that govern rhythmic motion of a highly articulated system, and to examine the onset of soot in counterflow laminar systems operated under (partial) premixed burning in a high-pressure (5 MPa) regime of relevance to compression ignition (CI) engines.. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Thomas Daniel, University of Washington; *Muscle's Energetic Versatility Arises From Its Crystalline and Multi-Component Structure*
- Professor Avinash Dongare, University of Connecticut - Storrs; *Scaling Relationships for Mesoscale Modeling Of Dynamic Failure in Titanium and Titanium Alloys*
- Professor Earl Dowell, Duke University; *Statistical Energy Analysis and Asymptotic Modal Analysis of Nonlinear and Nonconservative Engineering Systems*
- Professor Rebecca Fahrig, Stanford University; *A New Quantitative 3D Imaging Method for Characterizing Spray in the Near-field of Nozzle Exits*
- Professor Maria Fonoberova, AIMdyn, Inc; *Koopman Mode Decomposition Methods in Dynamic Stall: Reduced Order Modeling and Control*
- Professor Alessandro Gomez, Yale University; *Incipient Soot Formation in Rich Partially Premixed Flames under High Pressure Conditions of Relevance to Compression-Ignition Engines*
- Professor Jon-Paul Maria, North Carolina State University; *Rational Engineering of Reactive Nanolaminates for Tunable Ignition and Power*
- Professor Michelle Pantoya, Texas Technical University; *Characterizing Ignition, Combustion, and Energy Transfer from Composite Energetic Materials*
- Professor Harold Park, Boston University; *Nonlinear Dynamics of Electroelastic Dielectric Elastomers*
- Professor Anatoli Polkovnikov, Boston University; *Microscopic Approaches to Quantum Non-Equilibrium Thermodynamics and Information*

- Professor Laxminarayan Raja, University of Texas at Austin; RailPAc: *A Rail Electrode Based Plasma Actuator for High-Authority Aerodynamic Flow Control*
- Professor Shai Revzen, University of Michigan - Ann Arbor; *The Case for Morphologically Modulated Dynamics*
- Professor Andrew Spence, Temple University; NOFaLL: *Neuromechanics and Optogenetics: Dissecting Fast Legged Locomotion*
- Professor Ghatu Subhash, University of Florida - Gainesville; *Spatial Distribution of Amorphization Intensity in B4C during Rate-Dependent Indentation and Ballistic Impact Processes*
- Professor Kunihiko Taira, Florida State University; *Turbulent Flow Modification With Thermoacoustic Waves For Separation Control*
- Professor Eric Tytell, Tufts University; *Coupling Mechanical and Neural Properties for Effective and Adaptable Locomotion*
- Professor Choong-Shik Yoo, Washington State University; *Dynamic Response of Reactive Metallic Alloys*
- Professor Xiaolin Zheng, Stanford University; *Quantification of Ignition Properties of Porous Si Based Energetics*

2. Short Term Innovative Research (STIR) Program. In FY14, the Division awarded five new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to derive canonical distributions for non-equilibrium systems, develop a basis for understanding distributed mechanics and control of high-acceleration, high-precision multi-joint systems, and to identify the tradeoffs between distributed compliance, stiffness, actuation, and control in rapidly accelerating soft bodies. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Nikolaus Correll, University of Colorado - Boulder; *Exploring a Uniform Modeling Framework for Material-centric, Morphological Computation*
- Professor Adom Giffin, Clarkson University; *Determining Dynamical Path Distributions using Maximum Relative Entropy*
- Professor Daniel Goldman, Georgia Tech Research Corporation; *Principles Governing the Mechanics and Control of Snake Strikes*
- Professor Kenneth Kamrin, Massachusetts Institute of Technology (MIT); *Toward Theoretical Foundations of Resistive Force Theory of Granular-Structural Interaction*
- Professor Eric Tytell, Tufts University; *Neuromuscular Control of Rapid Linear Accelerations in Fish*

3. Young Investigator Program (YIP). In FY14, the Division awarded one new YIP project. This grant is driving fundamental research, such as studies to enable new real-time state estimation methods based on complex systems theory, non-probabilistic sensor fusion, and information theory. The following PI and corresponding organization were recipients of the new-start YIP award.

- Professor Jonathan Rogers, Georgia Tech Research Corporation; *State Estimation of Complex Dynamical Systems Using Information Theory*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY14 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *2014 Gordon Research Conference on Energetic Materials*; Newry, ME; 15-20 June 2014
- *2014 Princeton-CEFRC Summer School on Combustion*; Princeton, NJ; 22-27 June 2014
- *UMD Workshop on Distributed Sensing, Actuation, and Control for Bio-inspired Soft Robotics*; College Park, MD; 11-12 September 2014

5. Special Programs. In FY14, 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 three 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. Spray and Combustion of Gelled Hypergolic Rocket Propellants. Two MURIs in this topic area began in FY08. One team is led by Professor Stefan Thynell at the Pennsylvania State University, and the second team is led by Professor Stephen Heister at Purdue University. The objective of these MURIs is to understand the processes and mechanisms that control droplet formation, droplet collision and mixing, ignition, and energy release in gelled hypergolic propellants. The projects involve research in the areas of ballistic imaging, aerosol shock tubes, and ultra-fast laser diagnostics to capture reaction characteristics, and focus on fluid and gas dynamics, chemistry, chemical kinetics and reaction mechanisms, computational fluid dynamics with reactive chemistry, heat transfer, high-performance computing modeling and simulation, and advanced experimental diagnostic methods. The ultimate goal of the efforts is to gain understanding allowing for the science based design of gelled hypergolic propulsion injector and combustor systems. The pursuit of this research may also yield unexpected paths leading to the discovery of new concepts for hypergolic propulsion. The team led by Professor Thynell has developed an integrated research program comprising material science, chemistry, physics, and engineering to address various fundamental issues critical to the development of gelled hypergolic propellant (GHP) spray and combustion technologies for future rocket and missile propulsion systems. New techniques will be developed that will resolve the entire range of length and time scales (from atomistic to device levels). Emphasis will be placed on the microscale and macroscale processes that dictate the propellant interfacial dynamics and chemical initiation mechanisms, as well as the propellant atomization, mixing, and flame development. The team led by Professor Heister is investigating the rheological characterization of gelled propellants, non-Newtonian flow physics of gelled propellants, and the combustion physics of gelled hypergols.

2. 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.

3. 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.

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

No new starts were initiated in FY14.

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

No new starts were initiated in FY14.

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 FY14, the Division managed 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 PECASE winners for each calendar year are typically announced by the White House at the end of the fiscal year. However, the 2014 PECASE recipients had not yet been announced at the time this issue of ARO in Review was completed. 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 FY14, the Division managed 11 new DURIP projects, totaling $1.86 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 is serving 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. These approaches touch on several Mechanical Sciences Division research areas, including: 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. High Strain Rate Failure Modeling Incorporating Shear Banding and Fracture

Professor Haim Waisman, Columbia University, Single Investigator Award

The objective of this research is to develop a reliable high strain rate computational model that accounts for the formation of shear bands and dynamic fracture. The approach is to couple a shear band model with a phase field fracture model to account for both phenomena in a unified framework. The goal of the project is to develop a basic understanding of the physical and numerical behavior of the phase-field shear band model.

In FY14, several accomplishments were made, including, developing a strong form of the model from thermodynamic principles and enhancing the typical phase field models to account for material degradation due to inelastic work. The formulation has been implemented in a finite element code FEAP and is currently being extended to parallel processing units. Preliminary testing of one and two-dimensional numerical models showing improved failure modeling over a wider range of strain rates than either fracture of or shear band modeling has been accomplished (see FIGURE 1). The fracture only model is most appropriate at low strain rates and the shear band only model is most appropriate at higher strain rates. The combined model bridges between the two individual phenomenon models, which is extremely important for modeling the transition regime, which may be encountered in numerous real world phenomena. It should also be noted that in the range of strain rates where shear banding occurs readily, the failure strains of the shear band and the phase-field, shear band models match, but the post failure energy absorption for the shear band model is significantly higher than what would be expected, since this model cannot account for a shear band transitioning to a crack. The PI is now evaluating the numerical merits of the formulation, and detailed study of the sensitivity of the model to various parameters.

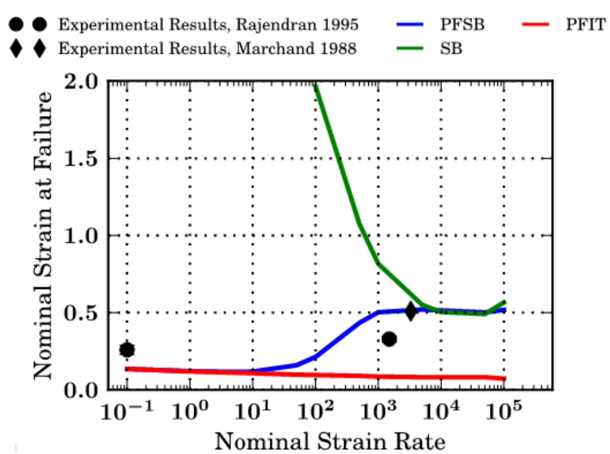

FIGURE 1

Failure strain vs nominal strain rate for a series of 1D simulations of steel. The blue curve shows the combined phase field + shear band model (PFSB), while the green and red curves model shear banding only (SB) and ductile fracture only (PFIT), respectively.

B. Peridynamic Models for Impact Damage and Brittle Fracture in Multilayered Protective Systems

Professor Florin Bobaru, University of Nebraska - Lincoln, Single Investigator Award

The objective of this research is to understand the progression of damage and failure in multilayered brittle protective systems induced by impact. Existing models have not been able to deliver predictive results in the complex failure of transparent/opaque protective systems (e.g., glass, ALON, SiC). Because in brittle systems material interfaces and use of graded or heterogeneous materials greatly influence its dynamic fracture response, the research team's objective is to develop models that are capable of accurately simulating the evolution of damage in such brittle systems. Computational models capable of predicting the dynamic fracture and fragmentation of brittle targets can help in the design of improved protective systems, including the use of tailored interfaces, graded and/or heterogeneous materials. The objective is being pursued through two main tasks. First the PI will develop peridynamic models that replicate the behavior of materials at high strain-rates given by equations of state for a specific material. The second task is to increase the efficiency of the peridynamic computation of dynamic brittle fracture by formulating Flux-Corrected Transport algorithms for the Peridynamic formulation in 2D and 3D. The current 1D FCT algorithms, developed in prior work, will first be extended to 2D followed by testing and verification.

Professor Bobaru's laboratory made several notable accomplishments in FY14. First, in the impact on the thin glass plate with a polycarbonate backing plate, the peridynamic model is shown to predict the types of crack systems observed in the experiments as well as their morphology (e.g., roughness on some crack surfaces, number of radial cracks reaching the boundaries of the sample). The researchers found that the radius of ring cracks produced near the impact center soon after impact match previously published theoretical and experimental results. These cracks are a result of the Rayleigh waves being reinforced by the longitudinal wave reflected from the boundary as a longitudinal wave and/or as a shear wave. Also, the longitudinal and shear wave emanating from the impact location do not create cracks by themselves. For example, radial cracks form behind the Rayleigh waves (which carry most of the elastic energy of the impact) while other types of cracks (e.g., circumferential, cracks parallel to the boundaries of the sample) are caused by wave interactions and reinforcement, primarily shear or Rayleigh waves colliding with reflected shear or reflected Rayleigh waves. All of these crack systems are found in the post-mortem sample/fragments in the experiments, at approximately the same locations as the crack systems computed with the peridynamic model. A number of cracks forming on the sides of the plate are caused by Rayleigh wave reflecting from the boundaries. The collision of the wave generated and travelling on the boundary of the sample and the incident Rayleigh wave creates failure spots that are spaced near the boundary of the sample. Some of these spots initiate cracks that run from the edge to the center (or edge-to-center cracks; E2C cracks). Fractography analysis performed in collaboration with ARL-WMRD confirmed these computational results. Finally, a similar plate of SiC is used instead of the glass plate in the simulations, with much higher bulk modulus, density, and almost 10-times the fracture energy of glass, crack patterns change significantly (see FIGURE 2).

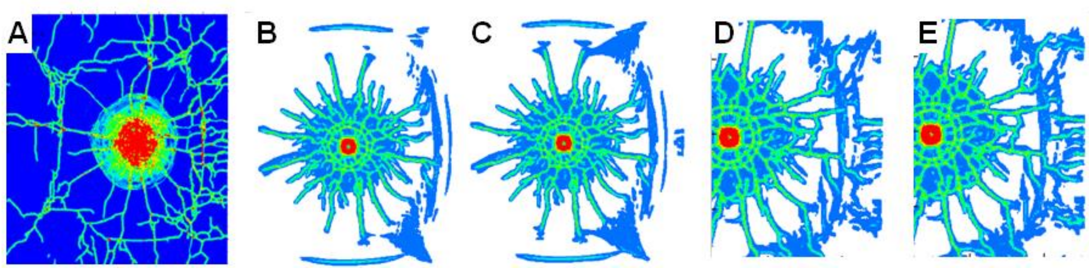

FIGURE 2

Evolution of damage in the impact on a thin glass plate. With plate size 10cm × 10cm × 3mm and impact at 150m/s, the panels show (**A**) the damage map of the impact side and back face of the glass plate, (**B-C**) a 3D view from the direction of impact of the regions that have some damage; notice the cracks that start on the right edge of the crack and move inward, and (**D-E**) zoom of portion of B-C at later timepoints; note more cracks forming on the right edge.

Additional results were found on the impact on a Functionally Graded Material (FGM) where the researchers found that the direction of variation of material properties slightly changes the crack propagation path and the duration of loading affects the propagation path in a dramatic way: under short impulse loading, the crack is "attracted" towards the strain energy concentration caused by a propagating Rayleigh wave, while under longer impulsive loadings, the crack propagates towards the point of application of the impulse, as it would do under quasi-static loading conditions.

Finally, in conducting work on the dynamic compressive tests on unidirectional FRCs the researchers found that under compression loading, the presence of defects can lead to both stable (such as matrix cracking) and unstable (fiber-matrix debonding and splitting cracks) crack growth. Also, depending on the alignment of the defect relative to the fiber direction and on the orientation of loading relative to the fiber direction, different failure modes are activated: matrix cracking and migrating over fibers, or fiber–matrix debonding.

C. Biological Locomotion Principles and Rheological Interaction Physics

Professor Daniel Goldman, Georgia Institute of Technology, Single Investigator Award

The goal of this research is to develop a program to discover principles of multi-mode biological and physical locomotion on and within wet and dry granular substrates. The work will build on the PI's previous work to discover principles of sand-swimming in dry granular media. The program will be composed of four research thrusts, each of which can operate separately but will ultimately interact: instrumentation development, biological studies, multi-body physical modeling and fundamental studies of intrusion into granular substrates. These will advance biomechanics, robotics, and the physics of complex media. For the Army, there is a need for robotic devices that can move effectively on and within complex ground like sand, soil and loose rubble. Such devices could perform military reconnaissance and urban search and rescue in such media by running and crawling on the surface, and even burying and swimming within it. In the biological world, many organisms such as soil, desert and beach dwelling lizards, snakes, crabs, scorpions and cockroaches are specialized to move in and on complex ground. Organisms use their locomotion capabilities to escape predators, regulate temperature, and hunt for prey. Existing robotic devices cannot match these organisms' multi-modal locomotor capabilities in complex environments.

Several novel research contributions were made in FY14. Chief among the PI's accomplishments is the discovery of the principles underlying agile limbless locomotion which appeared in the journal *Science* as well as *the Proceedings of the National Academy of Sciences*. Limbless organisms like snakes can navigate nearly all terrain. In particular, desert-dwelling sidewinder rattlesnakes (*Crotalus cerastes*) operate effectively on inclined granular media (like sand dunes) that induce failure in field-tested limbless robots through slipping and pitching. The PI's laboratory experiments reveal that as granular incline angle increases, sidewinder rattlesnakes increase the length of their body in contact with the sand. Implementing this strategy in a physical robot model of the snake enables the device to ascend sandy slopes close to the angle of maximum slope stability. Plate drag experiments demonstrate that granular yield stresses decrease with increasing incline angle. Together these three approaches demonstrate how sidewinding with contact length control mitigates failure on granular media. The PI also examined turning during sidewinding and replicated this motion for the first time in a robotic mechanism. Axial waves can provide a template for limbless organisms to simplify control of high-degree-of-freedom bodies, and modulation of these waves can produce a variety of locomotor behaviors. Sidewinding presents an interesting model system in which the combination of horizontal and vertical body waves may allow a greater versatility of turning behaviors by independent modulation of waves. The PI collected motion capture data from sidewinding rattlesnakes (*Crotalus cerastes*), and observed two distinct turning methods: "differential turning" and "reversal turning". In differential turning the research team observed an amplitude gradient in the horizontal wave component as it propagates down the length of the snake, causing one end of the snake to move further than the other over a single cycle. In reversal turning, the phase of the vertical wave rapidly changes by 180 degrees, causing an exchange of lifted and grounded body segments which results in a large net change of direction without significant body rotation. These hypothesized two-wave control mechanisms were applied to a modular snake robot which consequently replicated both differential and reversal turns on both sand and hard ground (see FIGURE 3). Further investigation into two-wave mixing parameters revealed a third turning mode, not used by snakes. These results show how the relative modulation of two component body waves can result in the emergence of complex behaviors and that high degree of freedom biological and robotic systems can be controlled and maneuvered using this simple control template.

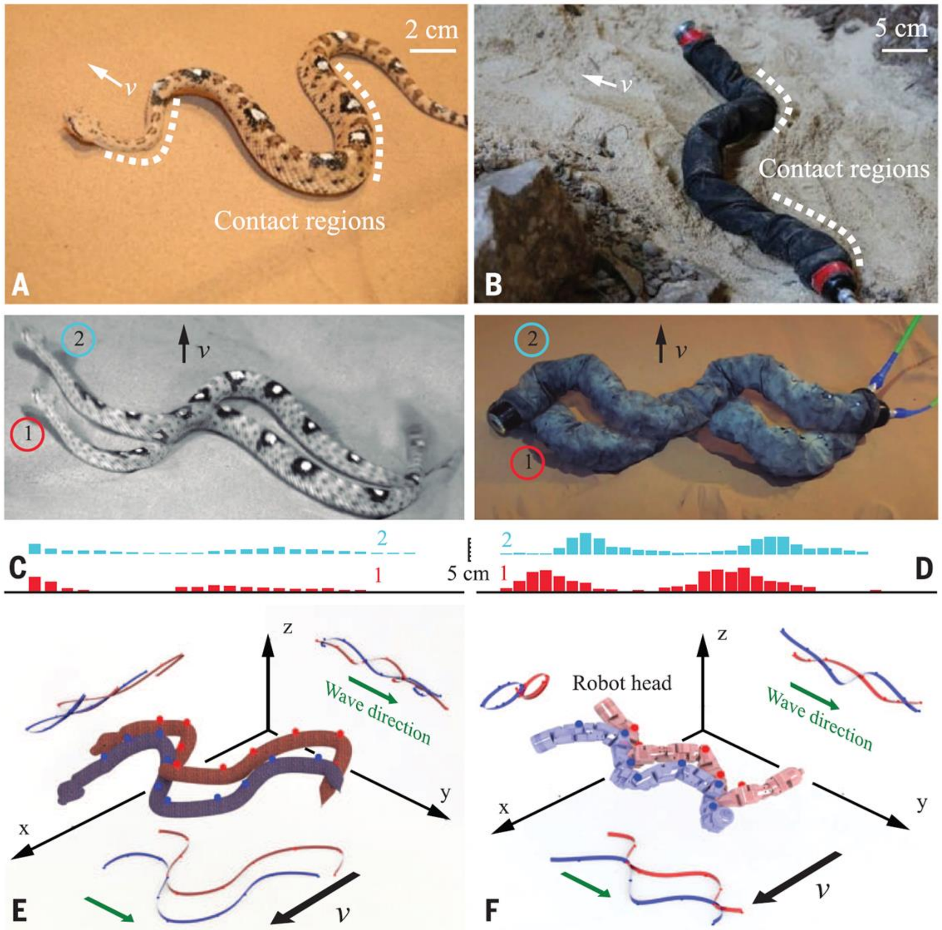

FIGURE 3

Sidewinding locomotion on granular media. (A) A Sidewinder rattlesnake (*Crotalus cerastes*) locomoting on a granular incline. The inset shows the experimental apparatus. (B) Robotic emulator traversing inclined granular media, similar to that in caves. (C) Two rendered snapshots of a snake sidewinding with red indicating the initial image and blue the successive image. The 3D configurations were reconstructed based on kinematics data the PI collected from a sidewinder rattlesnake moving on level ground. Shaded diagrams indicate centerline projections of the 3D reconstructed snake onto three orthogonal planes. (D) Snapshots of the robot performing sidewinding. The robot 3D configurations were reconstructed from wave kinematics used for sidewinding on level ground. The horizontal and vertical waves travel in the posterior direction of the robot (in the coordinate system attached to the robot).

D. Combustion of High Molecular Weight Hydrocarbon Fuels and JP-8 at Moderate Pressures

Professor Kal Seshadri, University of California - San Diego, Single Investigator Award

The objective of this research is to characterize combustion of high molecular weight hydrocarbon fuels and jet-fuels (in particular JP-8) and surrogates of jet-fuels in laminar non-uniform flows at elevated pressures up-to 2.5 MPa. Experimental and kinetic modeling studies are carried out. They include critical conditions of extinction and autoignition, and flame structure. Several scientific questions will be answered including: (i) How does pressure influence the critical conditions of extinction and autoignition? (ii) What surrogate best reproduces selected combustion characteristics of JP-8 at atmospheric and moderate pressure? (iii) What are possible chemical kinetic mechanisms for these surrogates? (iv) What are the influences of pressure on kinetic models of combustion of hydrocarbon fuels?

In FY14, accomplishments in both the experimental and kinetic modeling studies were achieved. In the experimental investigations of the influence of pressure on critical extinction conditions of laminar nonpremixed flames burning condensed hydrocarbon fuel, jet fuels, and surrogates study, the study of nonpremixed combustion of high molecular weight hydrocarbon fuels, jet fuels and surrogates, were carried out at pressures up to 0.4 MPa. The experimental study was carried out employing the counterflow configuration. In this configuration an axisymmetric stagnation-point flow of a gaseous oxidizer is directed downward and it flows over the surface of an evaporating pool of a liquid fuel. The counterflow burner used in this study was comprised of the liquid-fuel burner and an oxidizer duct. The liquid-fuel burner is made up of two parts: the bottom part comprises the fuel-cup, the exhaust system, and the cooling system, while the top part is the oxidizer duct. The counterflow burner and the oxidizer duct is placed inside the HPCEF. Liquid fuel was pumped to the fuel-cup. The amount of liquid fuel in the cup was maintained at a constant value by matching the mass rate of fuel flowing to the fuel-cup to the burning rate. Air diluted with nitrogen at 298K was injected onto the surface of the liquid. A flame was stabilized in the stagnation point boundary layer that is established above the liquid-gas interface. From an annular region that surrounds the fuel duct, a “curtain” flow of nitrogen flowed upward, and a cooling system surrounded this “curtain” nitrogen flow. Hot gases that were formed in the mixing-layer between the surface of the liquid pool and the oxidizer duct entered this cooling system. Reference fuels were tested, including n-heptane, cyclohexane, n-octane, iso-octane, and n-decane. Jet fuels tested included JP-8 and Jet-A. The surrogates tested were the Aachen surrogate, consisting of 80% n-decane and 20% 1,3,5-trimethylbenzene by mass, and the second-generation POSF 4658 Princeton surrogate consisting of 49.6% n-dodecane, 24.3% iso-octane, 19.8% n-propylbenzene, and 6.3% 1,3,5-trimethylbenzene by mass. The critical conditions of extinction of the Princeton surrogate agreed well with those of Jet-A, and JP-8 (see FIGURE 4).

A study of expected experimental accuracy of counterflow flame configuration was also conducted. Counterflow configurations are useful for investigating the structures of premixed, non-premixed, and partially premixed flames. Ignition and extinction conditions also are readily measured in this configuration. It was desirable to select an apparatus design that corresponded best to the conditions treated in available codes for calculating reacting flows because this facilitates comparisons of experimental and computational results. The most convenient codes to use are for steady laminar flows with one-dimensional scalar fields, and they often impose rotational plug-flow conditions at the boundaries. Accuracies of axisymmetric counterflow flame measurements in experiments intended to conform to these conditions were estimated for designs of large aspect ratios with straight-duct feed streams that have multiple-screen flow-smoothing exits. Causes of departures from assumptions underlying computational programs were addressed by methods that involve theoretical analysis, experimental measurement, and axisymmetric computation. It was concluded that experimental results would not be expected to differ from predictions made with plug-flow boundary conditions by more than five percent for properly designed counterflow experiments of this straight duct, multiple-screen type.

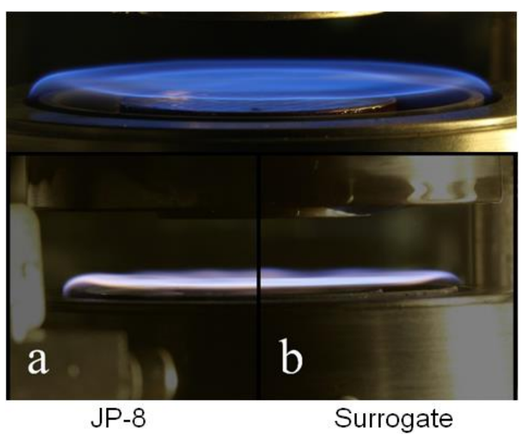

FIGURE 4

JP-8 vs surrogate combustion. Photograph of (**A**) JP-8 next to (**B**) surrogate B, the 2nd generation POSF 4658 Princeton surrogate. The flame was stabilized in the high pressure experimental facility for p = 0:25MPa, YO2;2 = 0:175, T_2 = 298K, and a_2 = 80s^{-1}.

E. Multiphase Combustion of Metalized Nanocomposite Energetic Materials

Professor Michelle Pantoya, Texas Tech University, Single Investigator Award

The objective of this research is to study stress state of aluminum particles and assess how manipulation of this property affects overall particle reactivity. Another objective is to resolve the exothermic surface chemistry associated with the phase of the alumina shell passivating aluminum particles and assess its impact on overall reactivity. The researcher is pursuing two main tasks. First, aluminum powders are being synthesized with affected shell stress to promote aluminum reactivity. This is being accomplished through controlled heating and cooling of the powder sample while stress is measured in-situ with an x-ray diffractometer. These powders will then be characterized for reactivity in a Digital Scanning Calorimeter-Thermal Gravimetric Analyzer. The second task is to examine surface chemistry between the alumina shell and halogen containing oxidizers. Powders synthesized as above with sizes under 25 microns will be treated to transfer the alumina from amorphous to gamma phase alumina. The shell phase will be confirmed with XRD and TEM. This "activated aluminum" will then be exposed to a fluorinated (or other halogenated) oxidizer and the surface chemistry kinetics analyzed with the DSC-TGA. Reaction quenching followed by TEM analysis will provide further information on the nature and rate of the resultant reactions. Surface functionalized aluminum particles will also be analyzed in a similar manner.

In FY14, several accomplishments were achieved. Continued work correlating electrostatic discharge (ESD) ignition sensitivity to electrical conductivity (i.e., a fundamental electrical property) of the Al particle core-shell structure matured into applying methods to desensitize highly sensitive powders to ESD stimuli thereby improving safety. Desensitizing an energetic powder was achieved by manipulating the electrical conductivity of the powder to a threshold on the order of 0.01 S/cm. This was accomplished by adding highly electrically conductive CNT particles. Percolation of the CNT was achieved for micron scale reactant powders with only 3 wt% CNT achieving an electrical conductivity of 0.03 S/cm and completely desensitizing the formulation to ESD stimuli while still enabling ignition with a thermal hot wire and enhancing energy propagation. For nano-scale Al particle mixtures, 13 wt% CNT was required to reach 0.05 S/cm and desensitize the mixture to ESD. The CNTs channel electrical energy through the particulate matrix preventing energy build up and ignition. The difference in required concentration is based on the geometry of the particulate media. Larger pore sizes in the micron scale media channel CNT particle connectivity requiring less to achieve percolation.

Ongoing investigations on the aluminum-fluorine surface chemistry are also being pursued. The research team examined the kinetics of fluorine based-acid coated Al particles, and is extending these investigations toward coatings that include highly viscous perfluoropolyether (PFPE) blended into nano-Al (see FIGURE 5). Their first study integrated this blend into polystyrene fibers via electro spinning to produce a ‘nanothermite fabric’. The metalized fibers were thermally active upon ignition from a controlled flame source with sustained flame speeds on the order of 2 mm/s varying as a function of blend loading. From this work, an operationally simple blendable approach to producing structural energetic composites loaded with PFPE coated n-Al particles yielded shape moldable, structurally flexible materials. Also, an epoxide system of poly(ethylene glycol) diglycidyl ether (PEG-DGE) and triethylenetetramine (TETA) were partially cured with n-Al/PFPE core-shell particles and mechanically mixed to produce a homogeneous composite material. With these two studies the potential for n-Al/PFPE blends is established and on-going investigations analyze fundamental interaction between PFPE and aluminum/alumina core-shell structures that control kinetics and reaction mechanisms.

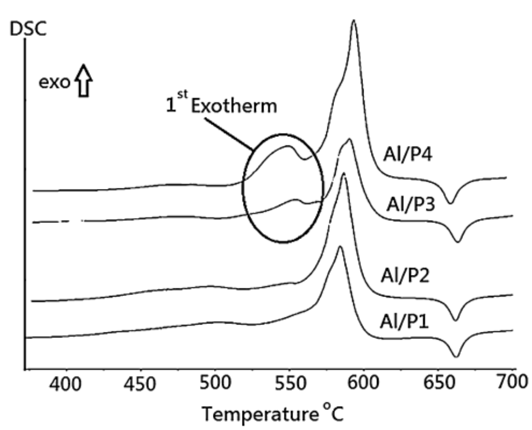

FIGURE 5

Heat flow as a function of temperature. Data plot for each composite of Al with PTFE with P1-P4 varying in chain length from smallest (P1) to largest (P4).

Exothermic surface chemistry on aluminum with polytetrafluoroethylene (PTFE) has also been investigated. PTFE particles synthesized for this study by DuPont vary with chain length and were combined with n-Al. Reaction kinetics were analyzed using DSC-TGA coupled with flame speeds. Results show a pre-ignition reaction (PIR) with longer chained PTFE samples and not with shorter chained PTFE samples (see FIGURE 5). The PIR is attributed to fluorine dislodging hydroxyls from the alumina surface and forming Al-F structures. Composites exhibiting the PIR correspondingly result in significantly higher flame speeds. These results help elucidate the influence of molecular scale surface chemistry on macroscopic energy propagation. Similarly, reaction kinetics of $Al+I_2O_5$ were also investigated and similar to fluorine, iodine was also found to produce a PIR on the alumina surface of n-Al particles.

A new approach has also been developed for depositing thin energetic films using blade casting. The reactant powders are bound together in films composed of polyvinylidene fluoride (PVDF) binder and methyl pyrrolidone (NMP). The on-going effort focuses on developing an understanding of controlling parameters promoting energy propagation in these flexible free-standing fluoropolymer based thermite films (see FIGURE 6). In particular, the rheology of the reactant mixture has been studied as shown in and the solids loading had an effect on flame speed. Very high solids loadings resulted in poor mixing and reduced flame speeds, whereas low solids loadings also resulted in reduced deposition density and thickness and were linked to reduced flame speeds. Also, flame speed increased as a function of film thickness, but calorific output was unchanged. Analysis of these results continues.

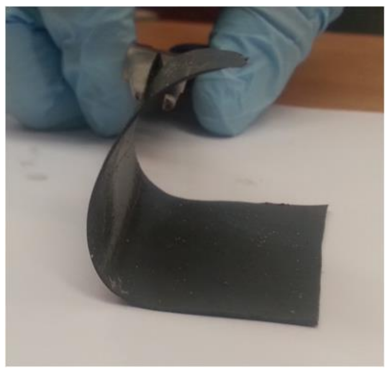

FIGURE 6

Flexible free-standing Al based thermite film.

Two-dimensional transient thermal images of aluminum/polytetrafluoroethylene (Al/PTFE) mixtures embedded with different additives were analyzed and the principal factors affecting the spatial temperature distribution during their combustion have been identified. Results showed two distinct temperature zones during combustion: a hot zone surrounding the point of ignition where the highest temperatures were recorded followed by a lower temperature region called the intermediate zone. Temperatures are plotted as a function of distance from the point of ignition such that inflection points distinguishing temperature gradients provide an indication of the range of the thermal influence. Results show greater gas generation in addition to condensed phase products promotes higher temperatures in the far field. Results also indicate that faster reactions attain higher temperatures and more extensive temperature fields. This observation is attributed to greater momentum of the gas and condensed phase products projected from the hot zone that shift the inflection point farther. These results revealed that multiphase convection is a governing mechanism promoting thermal energy distributions.

F. Hydrodynamic Flow Over Microtextured Surfaces

Professor Charles Maldarelli, The City College of New York, REP Award

The objective of this research is to investigate microfluidic flow phenomena along and through surfaces with topological features on the scale of tens to hundreds of microns. A validated modeling framework was developed to obtain hydrodynamic solutions for droplets and biomolecular microbeads corresponding to interactions with various microtextured topologies. The results of this effort were used to understand the fluid dynamic impacts on relevant kinetic interactions in a novel microfluidic cell that can be used for biomolecular screening.

In FY14, the researchers developed a microtextured surface consisting of traps ("V" shaped open enclosures), integrated as the bottom surface of a microfluidic cell, to form microbead arrays, and demonstrated the use of the cell as a device for screening the binding interactions of a "target" biomolecule against a library of "probe" molecules (see FIGURE 7). Sets of microbeads, with each set displaying a probe molecule attached to its surface, were streamed through the cell sequentially and entrapped by the microtextured surface to form the probe library. Although the traps could enable more effective lab-on-chip capabilities, the understanding of microtextured boundary layer flow effects on binding interactions with trapped microbeads has received little attention. Therefore, the researchers developed a multi-physics framework from theoretical considerations and compared hydrodynamic solutions, and kinetic solutions of the target mass transfer to the probes, with solutions of a "fictitious" untrapped microbead. The hydrodynamic solutions were formulated by the continuity and Navier-Stokes equations. Due to the low Reynolds numbers of the flow (~0.2), the motion is a predominantly a Stokes flow (i.e. viscous forces dominate inertia forces).

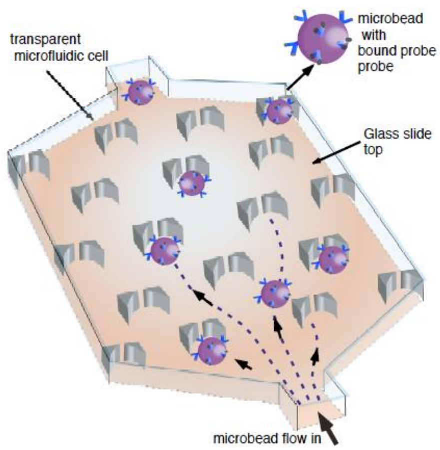

FIGURE 7

Microfluidic cell with microtextured traps for screening biomolecular binding interactions.

Hydrodynamic solutions for a representative unit cell with symmetry boundary conditions for the trapped and untrapped microbeads were compared for channels with heights and widths on the order of 100 and 1000 microns respectively, with average inlet flow velocity of 10-100 microns/s. Simulations for a Reynolds number of 0.2 showed that the presence of the traps has significant impact on the flow and the resulting mass transfer of the target to the probes (see FIGURE 8).

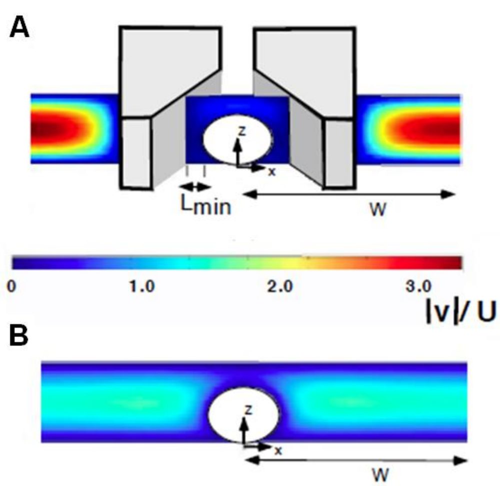

FIGURE 8

Simulation of the flow around a microbead. Simulations were performed for (A) trapped and (B) untrapped conditions. The magnitude of the normalized streamwise velocity (in the y-direction) is plotted in the x-z plane (i.e. plane with normal vector in the streamwise direction).

The researchers showed that the mass transfer occurs through a thin boundary layer around the microbead in regimes in which the target convective rate of transport along the microbead is large relative to the diffusive flux to the surface. Therefore, the surface shear rates (i.e., velocity gradients) are critical to understanding the target transport in the convective regime. For the gap on top of the microbead, the velocity is on the order of the mean flow and the corresponding shear rates are much larger than those for the lateral gaps in the trapped case. Therefore, the mass transport for the upper hemisphere of the microbead was shown to be larger than the lower hemisphere for the trapped case. In contrast, for the untrapped case, the shear rate in the top gap is comparable to that in the lateral gap, which would be expected to result in a much more symmetric mass transfer between the top and bottom hemispheres.

G. Investigation of the Flowfield Characteristics on a Retreating Rotor Blade

Professor Narayanan Komerath, Georgia Institute of Technology, Single Investigator Award

The objective of this research is to understand the reverse flow field features of rotors operating at high advance ratios (see FIGURE 9). There is a high level of uncertainty about the flow features which induce aeromechanically relevant effects, such as pitching moment loads and rotor stability in regimes that have been relatively unexplored in the past, but which are now of critical importance to the development of advanced high speed compound rotorcraft. Previous results on a teetering 2-bladed rotor in forward flight were extended to study high advance ratio (~1) flow fields. This effort represents the first to obtain public domain flow field velocimetry data for high advance ratio rotors dominated by reverse flow on the retreating side. Stereoscopic Particle Image Velocimetry (SPIV) was used to capture the 3-component velocity field in planes, and to investigate the researcher’s hypothesis of strong vortex formation under the blade in reverse flow and the influence of radial acceleration on the vortex.

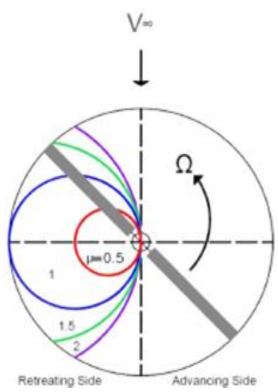

FIGURE 9

Contours of reverse flow regions for advance ratios from 0.5 to 2.

In FY14, a rotor experiment was used to capture flow field features at high advance ratios and to compare with a static blade (i.e. not spinning) in reverse flow in order to understand the effect of rotation in this regime. Particle image velocimtery data for the retreating side rotor flow field shows the formation of a sharp edge vortex formed on what is conventionally considered as the trailing edge of a blade (see FIGURE 10). Comparisons to a similar case for a non-rotating blade suggest that the rotation delays the formation of the vortex. The researchers also showed that the circulation associated with this vortex is substantial enough to contribute to blade loads such as lift force and pitching moment.

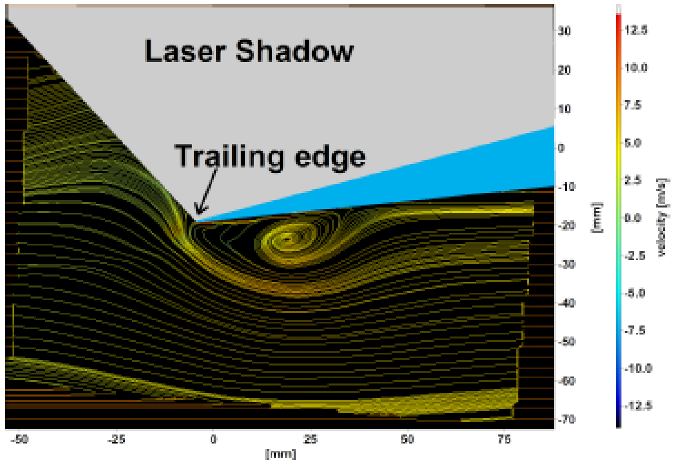

FIGURE 10

Velocity field under the rotating blade in reverse flow. Azimuth angle is 285 deg., 50% spanwise station, advance ratio is 0.8.

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 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: DARPA, Boeing Corporation, Teledyne Corporation

The objective of this research is to develop an efficient and accurate multiscale computational methodology for rapid virtual testing of composites with complex microstructures. The research goals include: (i) development of new 2D and 3D Adaptive Finite Element Model (A-FEM) elements that can explicitly account for statistical material heterogeneity and can faithfully predict progressive damage initiation, propagation and multi-crack interaction, and (ii) apply the new method to study composites of interest to the Army, coupled with 3D micro-CT-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.

The thermal-mechanical A-FEM (with steady-state and transient temperature DoFs) program has transitioned to several new research partners. Boeing and Teledyne are further developing and applying it to serve as a powerful materials processing/development module. The University of Miami researchers initiated a collaboration with both Boeing team and Teledyne team to integrate the A-FEM model into the work sponsored by the DARPA Materials Development for Platforms program which seeks to reduce applied material development time by a factor of four.

B. Studies of ARO-Relevant Fuels using Shock Tube/Laser Absorption Methods

Investigator: Professor Ronald Hanson, Stanford University, Single Investigator Award
Recipient: Air Force Research Laboratory - Aerospace Systems Directorate

The objective of this research is to study Army relevant fuels and surrogate fuels using recently developed shock tubes and laser absorption methods. This is expanding the current kinetics database of multi-species time-history measurement to Army relevant fuels and ignition conditions. The PI is using a newly developed high-pressure aerosol shock tube (developed under an ARO DURIP) to study ignition of aerosolized heavy hydrocarbon fuels at pressures of up to 100atm, while maintaining low temperatures (700K). This is a first of its kind exploration into ignition of heavy fuels at these conditions. The effort is also developing a new constrained reaction volume technique which will suppress remote ignition phenomena and generate a near-constant pressure reflected shock condition to generate near perfect data for use in models and model verification.

In FY14, the researchers transitioned the high pressure, long-test-time shock-tube methodology and design as well as methodologies for multi-species time-history measurements to the Air Force Research Laboratory Aerospace Systems Directorate and its research contractor, Universal Technology Corporation. These methods are being used to study the chemical kinetics of Alcohol-to-Jet fuels currently under development by AFRL.

C. Coherent Self-Sustaining Dynamics in High Dimensional Nonlinear Systems

Investigator: Professor Antonio Palacios, San Diego State University, Single Investigator Award
Recipients: U.S. Navy Space and Naval Warfare Center; Aviation and Missile Research, Development and Engineering Center (AMRDEC)

The goal of this research is to develop theoretical and computational methods in bifurcation theory and dynamical systems, general enough, to study a broad range of high-dimensional nonlinear systems in science and engineering. In particular, the research team seeks to uncover unifying principles by which they can analyze nonlinear interactions, at various length scales, and to use those principles to determine the conditions for the existence and stability of coherent self-regulated, self-sustaining, collective behavior.

The PI recently transitioned computational algorithms for exploiting nonlinear behavior in networks of nonlinear oscillators that will enable increased sensitivity for magnetic and electric field sensors. DoD scientists at Space and Naval Warfare Center used the new results to determine selection mechanisms for novel patterns of nonlinear behavior to enhance sensitivity in two types of technologies comprised of coupled bistable oscillator networks: fluxgate magnetic field sensors and signal channelizers. The underlying basic science was published in two journal papers that were jointly co-authored by the DoD and academic teams, with one article being selected as a special feature and cover story. AMRDEC researchers, in addition to developing tools for nonlinearity-enhanced sensitivity in non-GPS inertial measurement and guidance, are extending the methodology to enable the analysis of phase shifting arrays of chaotic oscillators, information flow in networks, and Boolean chaos.

D. Hydrodynamic Flow Over Microtextured Surfaces

Investigator: Professor Charles Maldarelli, The City College of New York, REP Award
Recipient: ExxonMobil Research and Engineering Company

The objective of this research is to investigate microfluidic flow phenomena along and through surfaces with topological features on the scale of tens to hundreds of microns. A validated modeling framework was developed to obtain hydrodynamic solutions of droplets and biomolecular microbeads due to interactions with various microtextured topologies. As part of this effort, the researchers have developed a microtextured microfluidic cell, which allows the *in situ* study and visualization of the electrocoalescence of a monodisperse emulsion of water droplets in oil. A uniform electric field applied across the emulsion polarizes the droplets creating dipolar attractive forces, which cause the coalescence.

The process developed by the researchers has drawn the interest of the oil industry for removal of water from oil, and transitioned to ExxonMobil through a collaborative research effort. As part of this collaboration, the researchers developed a microfluidic chip to study the process of electrocoalescence of water in oil emulsions in a crude oil. In the electrocoalescence process, an electric field is applied across an emulsion of water droplets in oil. The field polarizes the conducting water droplets in the insulating oil, creating dipole-dipole attractive forces which coalesce the droplets. This coalescence is used to remove water from oil. The microfluidic cell that was designed uses flow focusing to create a monodisperse emulsion of the droplets in an oil chamber in a transparent cell, and follows the electocoalescence process visually, through optical microscopy in the chamber as a field is applied across the droplets by electrodes placed on opposite ends of the chamber. The microfluidic design allows a visual picture of the electocoalescence process through the normally opaque crude oil because the height of the microfluidic chamber is small, of order 100 microns, and the monodisperse size distribution allows for a reproducible study. A theoretical framework and corresponding numerical discretization was developed to model the coalescence process, in which the electrostatic field equations in the emulsion are solved. This computation is done directly on the configuration of the droplets in the emulsion as obtained from the optical micrographs. From a map of these forces, evaluated on a pairwise basis, predictions are made as to which droplets coalesce based on whether the force is attractive (relative alignment of the droplets along the field) or repulsive (side alignment relative to the field), and these predictions are shown to agree with the observed coalescence process. The cell can be used to identify field strength conditions necessary to electrocoalesce the water droplets in a particular crude, and to identify surfactant promotors for the particular crude, which can accelerate the process.

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. Spatial Distribution of Amorphization Intensity in B_4C during Rate-Dependent Indentation and Ballistic Impact Processes

Professor Ghatu Subhash, University of Florida - Gainesville, Single Investigator Award

The objective of this research is to study boron carbide to evaluate the size and shape of the amorphized zone beneath indentation and impact surfaces of boron carbide by systematically varying the indentation load (10-1000 g), indentation rate (0.001 -5000/s), impact velocity (50-700 m/s) and impactor type (ball and rod). The objective will be achieved utilizing a novel polishing procedure to remove submicron depths of material from the loading surface and then probing each polished surface for amorphization peaks using micro Raman spectroscopy. In this manner, the entire subsurface volume of the indented (and impacted) region is fully mapped to obtained the severity and spread of the amorphization zone beneath each event. These maps are stacked together to obtain a spatial distribution of amorphized zone beneath the loading surface. Generating such 3D maps as a function of indentation load, indentation loading rate, impact velocity, and impactor type assists in gaining a better fundamental understanding of the evolution of the amorphized zone beneath a ballistic event. Based on this information a mechanistic-based model for critical stress required for initiation of amorphization and its size as a function of pressure and strain rate will be developed. It is anticipated that in FY15, static and dynamic indentations will be completed and Raman mapping of the amorphized zone will be initiated for the 300 g, 500 g and 1 kg loadings.

B. Investigating New Effects in Nanostructures: Pyro-electricity and Para-electricity

Professor Michael McAlpine, Princeton University, Single Investigator Award

Various approaches for thermal to electric power conversion have been investigated, including the Seebeck effect and pyroelectricity. However, methods exploiting heterogeneities in the mechanics of heterostructure materials and systems have not been explored to date as a viable means for investigating thermo-mechanical responses. The PI is currently focusing on two innovative mechanisms for investigating this area, based on the PI's discovery of two new phenomena which appear to have not previously been explored in either bulk or nanoscale materials. The first effect, called "pyro-paraelectricty," consists converting a thermal input into an electrical output in dielectric materials which exploit heterogeneities. The other effect that to be investigated is one the PI refers to as "pyro-flexoelectricity." The difference between this effect and "pyro-paraelectricity" is that the heterogeneous material system involved in the latter effect consists of rigid materials, thereby clamping the mechanical response such that the effect is due to changes in permittivity with temperature. By contrast, in "pyro-flexoelectricity," the heterogeneous system consists of a flexible substrate, such as a thin stainless steel, upon which a high permittivity insulating layer such as a BST film is sputtered. Thus, in this effect, a thermal input induces changes in curvature in the system due to differences in relative thickness and thermal expansion coefficients of the films, leading to bending. This subsequently leads to a flexoelectric response, in which a polarization is generated and hence an electrical output. These are two fundamental power conversion effects appear to be completely new. It is anticipated that in FY15 the research team will develop a detailed understanding of the mechanics and electronics of each phenomenon.

C. Dynamic Response of Reactive Metallic Alloys

Professor Choong-Sik Yoo, Washington State University, Single Investigator Award

The objective of this research is to understand the dynamic responses of reactive metallic alloys (RMA) -- how they deform, fracture and combust; how they evolve structurally and chemically to metal oxides and intermetallic products; and how they release chemical energy under thermal and mechanical loadings. The PI will perform several real-time optical/spectroscopic and synchrotron x-ray diffraction experiments and will investigate the dynamic thermo-mechano-chemical responses of RMA in atomistic and single-particle scales. Measurements will be performed on RMA in advanced nm-scale microstructures such as bulk metallic glass, lamellae multilayers, and high-pressure cold-sintered mixtures of constituting metals with high heats of combustion (such as Zr, B, Al, Ni, Ti, Hf, and Ce). The samples will be subjected to laser ablations or mechanical impacts in order to probe: fragmentation mechanics and fragments combustion of RMA subjected to laser ablations and mechanical impacts in controlled aerobic and anaerobic conditions, using time-resolved multi-channel optical pyrometry; structural and chemical evolutions through multi-scale reaction zones, using time-resolved synchrotron x-ray diffraction and time-resolved optical spectroscopy; dynamics of chemical energy release governing impulse characteristics, using high-speed, single particle micro-pyro-photography. It is anticipated that in FY15 experiments for RMA particle size studies for bulk metallic glasses (BMG) will be completed, as well as for nanomatallic mixtures and mass and temperature burn-rate measurements for combusting BMG in air.

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. Larry Russell, Jr.
Program Manager (Acting; Outgoing), Solid Mechanics

Dr. Asher Rubinstein
Program Manager (Incoming), Solid Mechanics

Dr. Bryan Glaz
Program Manager (Acting; Outgoing), Fluid Dynamics

Dr. Matthew Munson
Program Manager (Incoming), Fluid Dynamics

B. Directorate Scientists

Dr. Thomas Doligalski
Director, Engineering Sciences Directorate

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. Pamela Robinson
Administrative Support Assistant

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 2014* is to provide information on the programs and basic research supported by ARO in fiscal year 2014 (FY14), and ARO's long-term vision for transitioning 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 FY14.

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. In addition to advancing worldwide knowledge and understanding of networks, the research efforts managed in 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 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 FY14, 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 FY14 were $57.3 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY14 ARO Core (BH57) program funding allotment for this Division was $5.8 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 $5.5 million to projects managed by the Division. The Division also managed $44.4 million of Defense Advanced Research Projects Agency (DARPA) programs, and $0.2 million provided by other Army Laboratories. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.9 million for contracts. Finally, $0.5 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes 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 FY14 (*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 FY14 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 FY14, the Division awarded 19 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to examine specific aspects of communication to understand team-level processes and group performance, discover what the role of optimism and confidence play on the efficacy of learning in the presence of unawareness in game and decision theory, and to create theoretical methods, modeling approaches, and computational algorithms for co-evolutionary network dynamics, influence, and control. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Leman Akoglu, SUNY at Stony Brook University; *Anomaly Detection and Description in Complex Dynamic Networks*
- Professor Luis Amaral, Northwestern University; *Adoption of Innovations in Work Networks*
- Professor Rick Blum, Lehigh University; *Impacts and Mitigation of Attacks on Sensor Networks*
- Professor Carter Butts, University of California - Irvine; *Advancing Statistical Methods for Analysis of Multiple Networks*
- Professor Pamela Cosman, University of California - San Diego; *Video Transmission over Tactical Mobile Multihop Networks*
- Professor Wei Gao, University of Tennessee - Knoxville; *SAMAN: Social-Aware Mobile Adaptive Networking at the Tactical Edge*
- Professor Ashish Goel, Stanford University; *Algorithms, Mechanisms, and Platforms for Crowdsourced Democracy and Group Decision Making*
- Professor Carla Gomes, Cornell University; *Crowd Sourcing for Scientific Discovery*
- Professor Joseph Halpern, Cornell University; *Learning, Awareness, Optimism, and Confidence*
- ProfessorRobert Heath, Jr., University of Texas at Austin; *Millimeter Wave Mobile Ad Hoc Networks*
- Professor John Hopcroft, Cornell University; *Mathematical Foundations for Network Science*
- Professor Leslie Kaelbling, Massachusetts Institute of Technology; *A Belief-Space Approach to Integrated Intelligence*
- Professor Ying-Cheng Lai, Arizona State University; *Compressive Sensing for Nonlinear and Complex Systems Identification, Prediction, and Control*

- Professor Julio Mateo, 361 Interactive, LLC; *Linguistic Markers of Rapport and Cooperation in Team Communication*
- Professor Kamesh Munagala, Duke University; *Information Dynamics in Networks*
- Professor Todd David Murphey, Northwestern University; *Ergodic Control for Optimal Information Acquisition*
- Professor Jeff Shamma, Georgia Tech; *Coevolutionary Complex Networks: Dynamical Foundations, Influence, and Control*
- Professor Ness Shroff, Ohio State University; *Exploiting the Multi-Channel Advantage for Wireless Ad Hoc Networks: Achieving both High Throughput and Low Delay with Low-Complexity Control*
- Professor Pramod Viswanath, University of Illinois - Urbana; *Wireless Networks as Polymatroidal Graphs: Embedding, Multicommodity Flows, Cuts and Function Computation*

2. Short Term Innovative Research (STIR) Program. In FY14, the Division awarded four new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to investigate the role of abstraction and the use of double-oracles to address scalability problems in a class of Game theoretic solutions and to create network theoretic abstractions of coherent structures emerging in unsteady fluid motions. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Christopher Kiekintveld, University of Texas - El Paso; *Scalable Algorithms Based on Abstraction for Adversarial Reasoning under Uncertainty*
- Professor Sanjay Shakkottai, University of Texas at Austin; *Network Topic Modeling*
- Professor Yoav Shoham, Stanford University; *A Game Theoretical Approach to Practical Problems*
- Professor Kunihiko Taira, Florida State University; *Network-Theoretic Modeling of Fluid Flow*

3. Young Investigator Program (YIP). In FY14, the Division awarded six new YIP projects. These grants are driving fundamental research, such as studies to extend exponential random graph models to perform dynamic network analysis, prediction, and simulation, and to create intelligent systems that can establish operator and institutional trust by providing an interpretable summary of what they believe in and why. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor Zack Almquist, University of Minnesota - Minneapolis; *Scalable Temporal Network Models with Population Dynamics: Estimation, Simulation, and Prediction*
- Professor Dhruv Batra, Virginia Polytechnic Institute & State University; *Robust Reasoning Under Uncertainty: Building Reflective, Transparent, and Integrated Intelligent Systems*
- Professor Georgios-Alex Dimakis, University of Texas at Austin; *Learning Network Properties through Low Rank Approximations*
- Professor Devi Parikh, Virginia Polytechnic Institute & State University; *Robust Reasoning Under Uncertainty: Semantic Characterizations of Failures and Beliefs of Machine Perception Systems*
- Professor Chris Riedl, Northeastern University; *Social Network Processes in Collaborative Decision-Making*
- Professor Brooke Welles, Northeastern University; *Measuring "Network Thinking" and its Impact on Individual and Team Performance*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY14 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*; Evanston, IL; 4-6 December 2013
- *Cooperative Team Networks Workshop*; Berkeley, CA; 2 June 2014
- *NetSci 2014*; Berkeley, CA; 2-6 June 2014
- *Workshop on Wildlife Crime: An Interdisciplinary Perspective*; Washington, DC; 1-2 July 2014
- *Robotics: Science and Systems Conference*; Berkeley, CA; 12-16 July 2014
- *Control and Dynamical Systems (CDS) Workshop: Future Directions in Control, Dynamics, and Systems*; Pasadena, CA; 5-7 August 2014

5. Special Programs. In FY14, 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 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. Neuro-Inspired Adaptive Perception and Control. This MURI began in FY10 and was awarded to a team led by Professor Panagiotis Tsiotras of the Georgia Institute of Technology, with participation from researchers at the Massachusetts Institute of Technology and the University of Southern California. The objective of this MURI is to investigate a new paradigm based on "perception/sensing-for-control" to achieve a quantum leap in the agility and speed maneuverability of vehicles. The team will leverage attention-focused, adaptive perception algorithms that operate on actionable data in a timely manner; use attention as a mediator to develop attention-driven action strategies (including learning where to look from expert drivers); analyze the saliency characteristics of a scene to locate the important "hot-spots" that will serve as anchors for events; make use of fused exteroceptive and proprioceptive sensing to deduce the terrain properties and friction characteristics to be used in conjunction with predictive/proactive control strategies; and will study and mimic the visual search patterns and specialized driving techniques of expert human drivers in order to develop perception and control algorithms that will remedy the computational bottleneck that plagues the current state of the art.

This MURI will have significant benefits for the Army in the field and off the field, such as increasing vehicle speed and agility in direct battlefield engagements, as it will increase the chances of evading detection by the enemy or of escaping an ambush. As confirmed by several Army studies, the difficulty of successfully engaging and hitting a target increases disproportionately with the target speed. Support logistics will also become safer and more effective as even moderate increases in speed can largely increase the capacity of convoys and the throughput of the supply lines of materiel. Finally, the results of this research will contribute to the development of realistic off-road high-speed simulators for training special forces and other military and government personnel.

2. 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 scheduling of resources for ISR and for monitoring of contracts while building nations or societies.

3. 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.

4. 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.

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 FY14, 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

No new starts were initiated in FY14.

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 FY14, the Division managed 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

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each calendar year are typically announced by the White House at the end of the fiscal year. However, the 2014 PECASE recipients had not yet been announced at the time this issue of ARO in Review was completed. 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 FY14, the Division managed six 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. DARPA Anomaly Detection at Multiple Scales (ADAMS)

The ADAMS program is an effort to understand how insider threats to an organization (such as Nadal Hassan or Robert Hansen) can be predicted based on changes in behavior of individuals, or a small group of people within an organization. At a technical level this program involves mining incredibly large graphs (based on normal human activity) in a manner that is cognizant of human behavior, which reduces to computational challenges in managing and reasoning of large datasets, statistical reasoning techniques to find black swans, and efforts to manage uncertainty in both data and reasoning techniques. This program is managed on behalf of DARPA through the Network Sciences Division, Intelligent Networks Program.

I. DARPA Structured Social Interactions Module (SSIM)

The SSIM program is an effort to discover what makes certain soldiers, policemen and ethnographers effective in new environments (*e.g.*, a different culture to their own) making them "Good Strangers." Typically, Good Strangers can operate in a new environment without upsetting the local population and are good at understanding social mores without being taught what they are. This program engages social scientists to identify physiological coping mechanisms and psychological characteristics of Good Strangers, and artificial intelligence experts to devise new Social Science cognizant computer-based simulation and training algorithms. This program is managed on behalf of DARPA through the Network Sciences Division, Intelligent Networks Program.

J. DARPA Social Media in Strategic Communication (SMISC)

The SMISC program is an effort to understand and control strategic communication that takes place over social media. Recent events in Madagascar, North Africa (especially the Arab Spring) and in Bangalore suggest that social media could and does play a major role in bringing together mobs and crowds in unpredictable ways. The SMISC program aims to develop solutions that could be used to understand development of memes over social media and potential techniques to influence the formation or dissipation of memes. This program is managed on behalf of DARPA through the Network Sciences Division, Intelligent Networks Program.

K. DARPA Big Mechanism

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.

L. DARPA SIGMA

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 very 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.

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. Learning, Dynamics, and Intervention in Large-Scale Social Networks

Professor Anima Anandkumar, University of California - Irvine, YIP Award

In social network analysis, there exist algorithms to find groups of individuals by their social ties, but few algorithms allow for partial membership in multiple groups, which is common in real social networks. The objective of this research is to understand the structure and temporal dynamics of large, high dimension social networks, and from this understanding, derive tools for analysis and influence of these networks. In FY14, the research led to algorithms that can identify the multiple groups to which individuals within a social network belong. Specifically, individuals are modeled as having partial membership in different groups. Then the network connectivity data is used to create a three dimensional tensor representation. Tensor decomposition is utilized to determine the groups and their membership. The algorithms have be tested on portions of Facebook, the DBLP computer science article co-author network, and Yelp data with good results when compared to ground truth (for Facebook and DBLP data). Tensor processing algorithms were also developed, which were used to reduce the algorithm's processing time and complexity. These algorithms have also been applied to other problems, such as determining multiple topics of articles based on word and phrase contents.

B. Group Intelligence

Professor Thomas Malone, Massachusetts Institute of Technology, Single Investigator Award

The objective of this research is to determine if the size of a group affects the performance of a group, especially in cognitive tasks. In FY14, Professor Thomas Malone, at MIT's Center for Collective Intelligence, led an exciting and novel area of research to understand how to measure and train group intelligence. His team developed a measure for group intelligence, c, analogous to the general intelligence test for individuals that predicts a group's performance on a wide variety of tasks (Woolley, et al., 2010). Examples of tasks include brainstorming uses for a brick, creating a logistical plan for a shopping trip, and discussing a moral reasoning problem. The team discovered found that the average and maximum intelligence of individual group members were only moderately correlated with the widely used generalized individual intelligence scale. Instead, group intelligence was found to be significantly correlated with social perceptiveness of group members, low variance in speaking turn-taking (computational analysis of recording communication among group members; see FIGURE 1), and the percentage of females in the group.

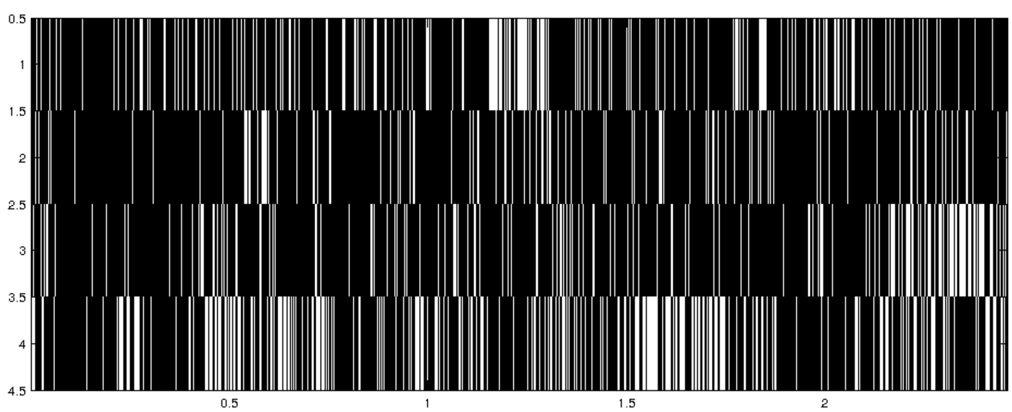

FIGURE 1

Turn-taking recordings indicate overlap and coordination of communication during group intelligence tasks.

The social perceptiveness scale is measured by a scale called "Reading the Mind in the Eyes" and detects people's ability to judge other's emotions from looking only at pictures only of their eyes. What is compelling about this finding is that it was replicated in studies using online group exercises, suggesting that this ability represents an underlying social capability that improves group members to coordinate and/or allocate resources effectively. This research has profound implications, suggesting that effective teams combine strong expertise as well as capabilities to perceive and coordinate the activities of others.

C. Control of Complex Networks

Professor Raissa D'Souza, University of California at Davis, MURI Award

The objective of this research is to understand and predict the properties of interdependent networks for the purpose of control. Collections of networks are at the core of military and civilian life, spanning technological, biological and social systems. All of these networks interact, leading to new emergent properties and unanticipated phase transitions and vulnerabilities. The research is divided into three main tasks, that bridge the team's collective expertise in statistical physics, information theory, control theory, systems reliability theory, animal behavior and experimental systems of NEMs oscillators. The research team made significant progress in FY14, with key accomplishments in three areas: (i) the use of graph products for network composition and decomposition to enable novel control schemes and provide basic models of interdependent critical infrastructure; (ii) Markov Chain models for analyzing network dynamics in systems as diverse as animal societies to networks of nation states, and (iii) novel random graph methods to analyze flows on networks as well as structural controllability properties. The researchers' advances in these areas are detailed below.

Graph Theory Advances. When dealing with collections of interacting networks, one has to move beyond representing a network as a simple matrix describing connectivity between elements. The research team called this "beyond the adjacency matrix." Significant progress has been made in the use of graph products, such as Cartesian products, to both compose simple networks into more complex interdependent network structures and to decompose complicated structures into more simple building blocks. Notably, the Cartesian product of two graphs preserves certain spectral properties of the individual graphs. Thus, if the individual graphs can be shown to be controllable, then it can be shown that the composite graph will also be controllable. This is provided that the composition process does not introduce symmetries absent in the atomic graphs (see FIGURE 2).

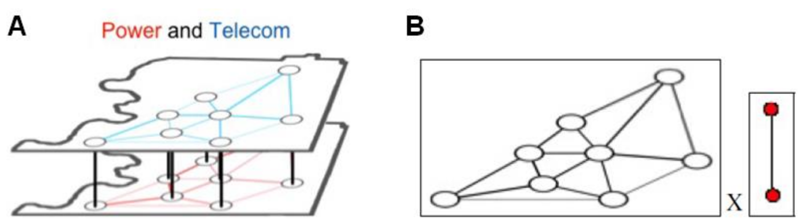

FIGURE 2

Advances in graph decomposition theory. (A) Schematic of co-located power and telecom hubs with similar network interconnections, which are approximated by the product of the two simpler graphs shown in (B). The controllability properties of the simpler graphs (B), enable analysis of the controllability of the complex, interdependent graph (A).

Markov Chain Model Advances. From the more theoretical, information theory side, the research team used Markov chain models to compute disparities in time scales intrinsic to a stochastic process and the observation of that stochastic process, allowing one to monitor how an observer synchronizes to properly extract meaningful information about stochastic dynamics. The researchers team studied the notion of using "spillover" effects for the purposes of control of interdependent networks. In this context spillover means that one can intervene in one network (or one network layer) and see collateral effects in another network (or network layer). Yet, how to measure spillover quantitatively was an open question. The MURI team developed statistically rigorous methods to quantify spillovers in multi-relational networks. The main challenge is that, with any system of networks, some correlation in the edge and node dynamics will exist due purely to random chance. Using Markov Chain analysis, the team was able to build an appropriate null model to correct for the noise arising from randomness and extract true correlations with empirical support from multiple data sets (see FIGURE 3).

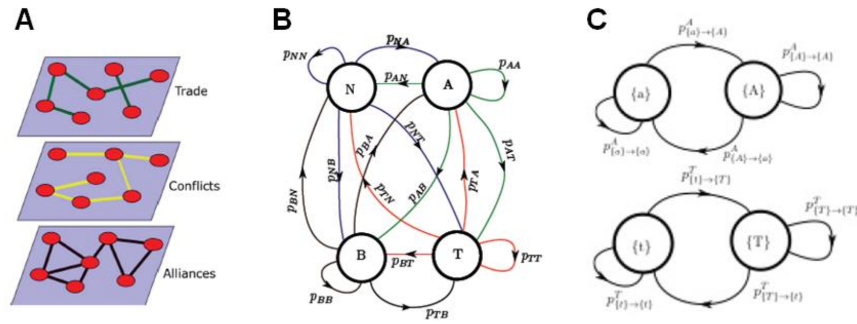

FIGURE 3

Markov chain modeling advances. (A) A multi-relational network of nation states, with layers of trade, conflict and alliance relations. (B) The state transitions and associated probabilities as observed in the real data of interrelated trade and alliance relations. (C) The null model which assumes the dynamics between the two layers are independent.

Random Graph Models and Structural Control Theory. Random graph models form a cornerstone for modeling the structure and function of real-world networks. They are idealized abstractions that allow one to analytically calculate network properties. This MURI made two important advances focused on network control. The first involves controlling self-organizing dynamics on networks (i.e., collective properties), the second involves predicting the onset of phase transitions. Control of a self-organizing system is particularly challenging, as the system responds to control actions in an unanticipated way. A quintessential model of "self-organization" is the Bak-Tang-Weisenfeld sandpile model of cascading failures. Although the model is a non-linear dynamical system, almost all mathematical analysis is conducted in the steady-state regime, where researchers have used this model to establish the well-received concept of "optimal interdependence" between systems. However, it is clear that steady-state analysis does not capture the system's behavior far from equilibrium and thus the dynamic response of the system to control interventions. In FY14, the team developed a zero-parameter model that captures the essential self-organizing mechanisms of sandpile cascades on networks. The team can now analyze the impact of control interventions. A significant result has also been achieved by establishing new markers of early-warning signs for the onset of phase transitions, where the team identified how "micro-transitions" (small statistical fluctuations) during the early evolution of a network show a discrete scaling behavior which allows us to build a recursion relation and predict the location of the network percolation phase transition. Knowing how to predict the location of a phase transition, well before the transition point, opens the door for a new family of control and intervention actions (see FIGURE 4).

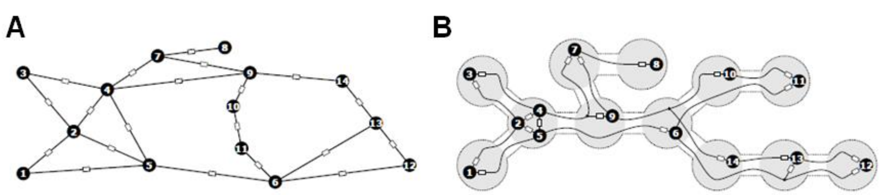

FIGURE 4

Random graphs and cascading failure intervention. (A) The IEEE 14 bus power flow test case and (B) the equivalent tree-width decomposition. The MURI team is building random graph models which plug together "wide motif" constituents to allow analysis of flows and cascading failures on networks with nested loops.

D. Computational and Mathematical Analysis of Tipping Points

Professor Chjan Lim, Rensselaer Polytechnic Institute, Single Investigator Award

The goal of this research is to investigate the interdependency between structure and dynamics of social networks, investigate how communities are formed in social networks, and to design robust algorithms for community detection. In prior work, the PI showed that in a large social network of agents with only two opinions A and B with the ability to simultaneously hold both, a 10% of committed diehards in the minority opinion A will achieve total consensus in times log in N, size of network, while committed fractions of less than 10% will take on average exp N time (which is practically indefinite) to achieve domination (*cf*. Xie, et al., 2011 and Zhang, et al., 2011). It is clear why sharpening this result in the direction of better estimates for the Tipping fraction on large random and scale free social networks could be useful to Army efforts in building societies. Consequently, the group made up of network science and nonequilibrium statistical physics experts improved on prior work by way of Coarse-graining and Random walk models in analyzing and simulating the effect of committed agents and central agency on time to consensus in a class of agent based network models (Naming Games, Voter Models). Two examples of recent results from this research are described below.

Exact Spectral Solutions for Diffusion-Dominated Signaling Games: Together with graduate assistant William Pickering, the PI has formulated a spectral method for the exact solutions of the canonical diffusion-dominated signaling games, Voter models, on a wide range of network topology. This method is based on the generating function approach to solving the spectral problem of the Markov Propagator in the Voter models, and was inspired by Kac's work in the 1940s on the Ehrenfest Urn Problem. Complete knowledge of the leading eigenvalues and eigenvectors of these problems yield a trove of bulk or averaged quantities that are sought after in the nonequilibrium statistical physics of this class of models. They include expected times to consensus and all their moments, the latter providing valuable information on the fluctuations or variance of consensus times under different runs of the same models from the same initial data. Furthermore, these moments of consensus times are all solved for the whole range of possible initial data for the models (such as starting fractions of opinions, etc.). The results have been made available in arxiv.[1]

Naming Games on Random Geometric Graphs – PDE methods. The PI investigated the two-word Naming Game on two-dimensional random geometric graphs. Studying this model provided an understanding of the spatial distribution and propagation of opinions in social dynamics. A main feature of this model is the spontaneous emergence of spatial structures called opinion domains, which are geographic regions with clear boundaries within which all individuals share the same opinion. The PI provided the mean-field equation for the underlying dynamics and derived several properties of the equation such as the stationary solutions and two-time-scale separation. For the evolution of the opinion domains the PI found that the opinion domain boundary propagates at a speed proportional to its curvature. Finally the PI investigated the impact of committed agents on opinion domains and found the scaling of consensus time.[2]

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[1] Pickering W, Lim C. (2014). Solution of the Voter models by Spectral Analysis. arXiv:1408.2130.

[2] Zhang W, Lim C, Korniss G, Szymanski B. (2014). Opinion Dynamics and Social Influencing in Random Geometric Graphs. *Scientific Reports*. 4:5568.

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 to external organizations and customers.

A. Application of Rateless Codes to MANETS

Investigator: Professor Mike Pursley, Clemson University, Single Investigator Award
Recipient: U.S. Navy Space and Naval Warfare Systems Command (SPAWAR)

The use of rateless codes for point-to-point wired and wireless links has been well established to reduce the overhead of retransmission. The goal of this research is to explore the use of rateless codes in unicast and multicast in a multi-hop scenario. Professor Pursley has taken these techniques and expertise on rateless codes developed during this research to advise the SPAWAR engineers on Joint Tactical Radio System waveform and coding design, development, and testing. This transition led to improved performance for DoD tactical radios.

B. Predicting and Controlling Cascading Failures in Interdependent Networks

Investigator: Professor Raissa D'Souza, University of California at Davis, MURI Award
Recipient: AMRDEC and CERDEC

Researchers as part of a MURI team at the University of California at Davis developed new understanding to predict and control the factors leading to cascading failures in interdependent networks. Predictive understanding and robust control of the variety of factors leading to rare cascading failures in critical interdependent networks is one of the greatest challenges in modern network science. To date, idealized abstractions using random graphs have enabled scientists to begin to study this problem in isolated networks.

Recently, driven by the need to provide tools for more realistic "network of networks," the MURI team has developed a model, backed by U.S. power grid data, which is capable of capturing self-organizing mechanisms underlying the generation of cascading failures. In particular, new results have established how small statistical fluctuations, known as "micro-transitions," provide new markers of early-warning signs for the onset, location, and scaling properties of cascading failures. Research is now focused on generalizing the mathematical framework and developing a new control theory around these principles. Knowing how to predict the location of a dangerous micro-transition well before the transition point opens the door for a new family of control and intervention actions to protect DoD networks. This research was transitioned to AMRDEC and CERDEC researchers developing algorithms for controlling complex networks as well as understanding how to protect DoD networks against malicious intrusion.

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. High Throughput, Low Delay in Ad-Hoc Networks by Exploiting Multiple Channels

Professor Ness Shroff, Ohio State University, Single Investigator Award

Military multi-hop wireless networks require high throughput at low delay in order to support the warfighter. In addition, algorithms must have low complexity so that the protocols can be implemented in real time. Existing algorithms have high complexity that grows exponentially with network size or only use a fraction of the available network capacity, reducing throughput, increasing delay, or both.

The goal of this research is to optimize simultaneously on all three dimensions: throughput, delay, and complexity. It is anticipated that in FY15, the research will leverage the flexibility offered by multiple channel capability from modern communications techniques. Multi-channel networking can be optimized for specific traffic and quickly adapt as communications load or channel conditions change. Extensions will be considered for multiple antenna configurations and utilizing time division as virtual channels.

B. Social Network Processes in Collaborative Decision Making

Professor Chris Riedl, Northeastern University, Young Investigator Award

Professor Chris Riedl is investigating the problem of effective team coordination and problem solving. In FY15, he intends to use an innovative combination of field studies and agent-based modeling to answer fundamental questions about how best to organize humans to solve difficult problems. He is exploring the two dominant modes of problem-solving strategies: collaboration and competition, while accounting for the nature of the problem to be solved, information sharing structures among agents attempting to solve the problem, and individual-level preferences of agents.

The investigator will implement a series of simulations and experiments in which agents/individuals attempt to solve complex tasks where individuals are exposed to a variety of treatments modifying (a) the amount and type of information shared, (b) the structure of the underlying communication network (which agent can communicate with which other agents; i.e., network topology), and (c) the level of complexity of the task. This research identifies social network processes across groups of competing and collaborating individuals and determines their impact on practices and performance of individuals, teams, and organizations. This research promises to make important contributions to the literature on contests, collaborative work, virtual teams, and crowdsourcing. Furthermore, this research contributes to a better understanding of the changing nature of work in which large groups of agents operate as self-organized systems, highly relevant to understanding how non-state agents coordinate and mobilize.

C. Causation Entropy in Complex Networks

Professor Erik Bollt, Clarkson University, Single Investigator Award

Modern technological progress has led to the production of a massive amount of data, from molecular biology to global climate, or even social interactions. A perhaps overlooked but fundamental problem is, how much reliable information can be gained from such "big-data" to better understand a complex system - a system of hundreds, thousands, or even millions of dynamically interacting components. The objective of this research is to explore the (dynamic) flow of information in a complex system at different spatial and temporal scales. In FY15, the PI will explore spatiotemporal and functional structures in complex systems from components of simple elements, how such structures emerge, how information flows, and how this occurs across scales. The PI will also develop a theory for information dynamics in "hierarchically efficient" dynamical networks, specifically between scales, therefore allowing the design of complex networked systems that "collectively" and "optimally" transfer information. A rigorous mathematical framework (optimal causation entropy) for causality inference in general dynamical systems will be extended to the domain of networked dynamical systems. The method will be benchmarked for synthetic networks of hundreds of nodes and shown to outperform currently available techniques such as Granger causality and transfer entropy.

D. Semantic Characterizations of Failures and Beliefs of Machine Perception Systems
Professor Devi Parikh, Virginia Tech, Young Investigator Program

Autonomous systems that depend upon Machine Learning, unfortunately, fail miserably when encountering new situations that they have not been trained on. In order to rectify such situations, or at least degrade gracefully, autonomous systems need to be endowed with the ability to reflect upon their internal status. In FY15, the PI will investigate the use of coarse-grained semantic characterization to explain why a system failed. In particular, the PI will investigate meta-level reasoning capabilities and beliefs of perception systems. The goal of this effort is a level of description of failure that can be used by other systems that depend upon the perception system, in the context of robotics, so that corrective actions can be taken.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Purush Iyer
Division Chief
Program Manager, Intelligent Networks

Dr. Kathryn Coronges
Program Manager (Acting; Outgoing), Social and Cognitive Networks

Dr. Edward Palazzolo
Program Manager (Incoming), Social and Cognitive Networks

Dr. Samuel Stanton
Program Manager (Acting), Multi-Agent Network Control

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 2014* is to provide information on the programs and basic research supported by ARO in FY14, and ARO's long-term vision for transitioning 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 FY14.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Physics Division supports research to discover and understand 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. Beyond advancing the world's understanding of exotic quantum physics and extreme optics, the 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, 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 Physics 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), the Joint Technology Office (JTO), and the Joint Improvised Explosive Device Defeat Organization (JIEDDO). These interactions promote a synergy among ARO Divisions and DoD agencies, and impact the goals and improve the quality of the Division's research areas.

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 FY14, 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 one, two or three dimensional 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 like liquid nitrogen or liquid helium. The cooling is accomplished with 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 atom holography, along with breakthroughs in understanding strongly-correlated materials and the ability 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: (i) Extreme Light and (ii) Meta-optics. 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 reactions 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. Short, intense pulses self-focus in the atmosphere until the intensity reaches the breakdown value where nitrogen and oxygen are ionized, creating a plasma. This new form of radiation 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 of these pulses 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 as a means to understand and compensate for loss.

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, decoherence 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 entails experimental demonstrations of quantum logic performed on several quantum bits operating simultaneously. 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 Computation and Communication 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 FY14 were $55.3 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY14 ARO Core (BH57) program funding allotment for this Division was $6.8 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 $11.6 million to projects managed by the Division. The Division also managed $14.2 million of Defense Advanced Research Projects Agency (DARPA) programs, and $21.9 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.3 million for contracts. Finally, $0.5 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.1 million of 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 FY14 (*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 FY14 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 FY14, the Division awarded 10 new-start SI research projects, in addition to active awards continuing from prior years. These grants are driving fundamental research, such as studies to understand the quantum dynamics of entanglement generation and propagation in trapped atomic ions, to explore the underlying physics of quantum criticality using complex oxide heterostructures, and to characterize a novel class of nonlinear photonic negative-index metamaterials. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Silke Buhler-Paschen, Vienna University of Technology; *Kondo Insulator Interfaces*
- Professor Gregory Fiete, University of Texas - Austin; *Emergent Non-Equilibrium Phenomena in Driven Correlated Materials With Strong Spin-Orbit Coupling*
- Professor Winfried Hensinger, University of Sussex; *Development of Microwave Ion Chip Entanglement Architectures for Quantum Technologies*
- Professor Paul Kwiat, University of Illinois - Urbana; *Advanced Quantum Sensing*
- Professor Christopher Monroe, University of Maryland - College Park; *Long Range Quantum Dynamics and Entanglement Propagation in Atomic Qubits*
- Professor Alexander Popov, Purdue University; *Coherent Nonlinear Nanophotonics*
- Professor Qimiao Si, William Marsh Rice University; *Spin-Orbit Coupling and Strongly Correlated Electrons at the Interfaces of Heavy Fermion Materials*
- Professor Susanne Stemmer, University of California - Santa Barbara; *Quantum Critical Behavior in Oxide Structures*
- Professor John Thomas, North Carolina State University; *Many-body Physics in Two-dimensional Fermi Gases*
- Professor Vladan Vuletic, Massachusetts Institute of Technology; *Novel States of Light and Matter Mediated by Collective Rydberg Excitation*

2. Short Term Innovative Research (STIR) Program. In FY14, the Division awarded five new STIR projects to explore high-risk, initial proof-of-concept ideas, including studies to explore novel electronic states by gating strongly correlated material and to explore entanglement in non-quantum systems. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Gleb Finkelstein, Duke University; *Engineering and Probing Pairs of Majorana Resonant Levels in Carbon Nanotube Quantum Dots*
- Professor David Goldhaber-Gordon, Stanford University; *Novel Electronic States by Gating Strongly Correlated Materials*
- Professor Joseph Thywissen, University of Toronto; *A Local Probe for Universal Non-equilibrium Dynamics*
- Professor Anthony Vamivakas, University of Rochester; *Untangling Classical Optical Entanglement*
- Professor Kevin Webb, Purdue University; *Optical Force Theory*

3. Young Investigator Program (YIP). No new starts were initiated in FY14.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY14 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 Heavy Fermion Materials and Quantum Phase Transitions*; Houston, TX; 9-11 December 2013
- *Mechanical Systems in the Quantum Regime Gordon Research Seminar*; Ventura, CA; 8-14 March 2014
- *Frontiers of Quantum Optics Symposium*; Pasadena, CA; 25-26 April 2014
- *From Ultrafast to Extreme Light Symposium*; Ann Arbor, MI; 22 June 2014
- *Correlated Electron Systems Gordon Research Conference*; South Hadley, MA; 22-27 June 2014
- *Quantum Information Science Gordon Research Conference*; Easton, MA; 26 July - 1 August 2014
- *24th International Conference on Atomic Physics*; Baltimore, MD: 8-13 August 2014
- *Structured Light in Structured Media from Classical to Quantum Optics*; Washington, DC; 29 September - 1 Oct 2014

5. Special Programs. In FY14, 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 one 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. Conversion of Quantum Information among Platforms. This MURI began in FY09 and was awarded to a team led by Professor Christopher Monroe at the University of Maryland. The objective of this MURI is to explore the conversion of quantum information from one form to another.

Since the inception of research in quantum information, a number of platforms have been explored to implement quantum information: trapped ions, ultracold atomic gases, semiconductor quantum dots, superconductors, and others. Each of these systems has a unique advantage while also suffering disadvantages in other areas. For example, trapped ions are relatively easy to manipulate and are readily isolated from the environment. However they cannot be readily scaled up to the size necessary for practical applications. Semiconductors are perfect for that, but the quantum information is too quickly lost to the surrounding material for a practical computation to occur. To address these matters, the MURI is considering the potential for converting quantum information from one platform to the other without losing the quantum nature of the information. In particular the intra-conversion of information between atomic systems, solid state systems, and optical systems is being explored. If the best of each platform can be combined and the detrimental problems avoided, then the development of quantum information capabilities will be accelerated. The advent of a quantum computer will provide solutions to problems that are computationally intractable on conventional computers, impacting resource optimization and improved logistical support.

2. Harnessing Electronic Phenomena at Oxide Interfaces. This MURI began in FY09 and was awarded to a team led by Professor Susanne Stemmer at the University of California - Santa Barbara. The objective of this research is to investigate the unexpected electronic effects found to exist at the interfaces of certain crystalline oxides.

Recent studies have shown that carefully designed and grown interfaces between different crystalline oxides can lead to electronic phenomena at that interface that are foreign to the oxides that form it. These studies have suggested the potential for a new type of electronics technology; therefore this new MURI aims to determine if these effects can be designed and controlled. The research focuses on the Mott transition: a metal-to-insulator transition that results from electron-electron repulsion. The objective is to design and control the oxide-oxide interface as a new approach to understanding, predicting and controlling the Mott metal-insulator transition and the associated electronic phenomena. The electronic energy states that determine the character of the material are tied to the metal-oxygen atom distance in the crystal and the crystal symmetries. Accordingly the team will construct alternating layers of a material containing a known Mott metal-insulator transition with an insulator that will affect the bonding distances and symmetry of the adjacent Mott material. The ability to control this transition may lead to new options for enhancing logic, memory and other technologies important for advanced computational capabilities.

3. 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).

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.

4. 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.

5. 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.

6. 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.

7. 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.

8. 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.

9. 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-dephosporylation 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.

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.

10. 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

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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.

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.

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

No new starts were initiated in FY14.

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 FY14, the Division managed two new-start Phase I SBIR contracts, in addition to active projects continuing from prior years. These 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 FY14, 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 PECASE winners for each calendar year are typically announced by the White House at the end of the fiscal year. However, the 2014 PECASE recipients had not yet been announced at the time this issue of ARO in Review was completed. 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 FY14, the Division managed seven 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. 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.

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. Ferroplasmons: Intense Localized Surface Plasmons in Ferromagnets

Professor Ramki Kalyanaraman, University of Tennessee - Knoxville, Single Investigator Award

The goal of this project is to understand ferroplasmons, which are strong plasmonic effects in ferromagnetic metals, and to understand the coupling of light and magnetism in ferroplasmonic materials. In FY14, the research team, led by Professor Ramki Kalyanaraman and collaborators Professor Gerd Duscher, Hernando Garcia, and Anup Gangopadhyay, made the first experimental demonstration of ferroplasmons in bimetallic nanoparticles made from a CoFe alloyin contact with silver (see FIGURE 1). Unlike the weak plasmonic signal in the pure ferromagnetic metal (see FIGURE 1E, dashed curve), bimetals with segregated regions of Ag and CoFe showed ferroplasmons with energies in the visible range (see FIGURE 1E, solid curve)] and intensities comparable to that of plamsons in silver, which is the best known plasmonic material.

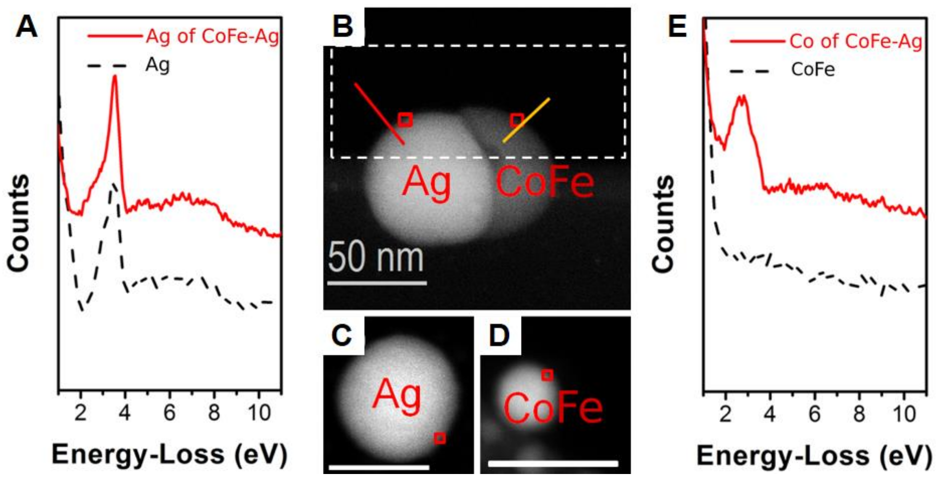

FIGURE 1

High resolution electron energy loss spectroscopy (EELS) leading to discovery of ferroplasmons.
(**A**) EELS signal from surface of pure Ag (dashed curve) vs Ag in Ag-ferromagnet bimetal. (**B**, **C**, **D**) Ag-ferromagnetic bimetal, pure Ag and pure ferromagnetic nanoparticles, respectively. The scale bars in (**C**) and (**D**) correspond to 50 nm. (**E**) EELS signal from surface of pure ferromagnet (dashed curve) and for ferromagnet in contact with Ag (solid curve) showing clear evidence for a ferroplasmon signal.[5]

To understand the origin of the ferroplasmons, detailed mapping of the near field plasmonic behavior was performed with state-of-art electron microscopy and extremely high-resolution (<0.1 eV) EELS analysis. By probing the surface and bulk of the nanoparticles, The PI constructed the first exhaustive plasmon map that helped construct a plasmon energy diagram (see FIGURE 2). From such studies it became evident that the ferroplasmon is not due to leakage of plasmonic energy from the Silver into the Cobalt metal, as has been known previously from magneto-optical studies of noble metal-ferromagnetic systems. Instead, the ferroplasmon appears to be due to a strong electromagnetic interaction between the two metals. Their preliminary hypothesis based on theoretical modeling suggests that a plasmon coupling scheme such as dipole-dipole interaction or plasmon hybridization could generate novel plasmons in the ferromagnet. Quantitative predictions will require a careful investigation of the role of the interface (for example the metal-metal contact potential) and is presently underway.

[5] Sachan R, Malasi A, Ge J, Yadavali S, Krishna H, Gangopadhyay A, Garcia H, Duscher G, and Kalyanaraman R. (2014). Ferroplasmons: Intense Localized Surface Plasmons in Metal-Ferromagnetic Nanoparticles. *ACS Nano*. 8:9790-9798.

The PI's discoveries were highlighted in a perspective article in ACS Nano published by international experts.[6] In the perspective, the ferroplasmon was highlighted as a potential new approach for magneto-plasmonic data storage. The authors also performed FDTD analysis of non-contacting Ag and Co spheres which suggests that their hypothesis of an electromagnetic interaction between the metals could be responsible for the ferroplasmons.

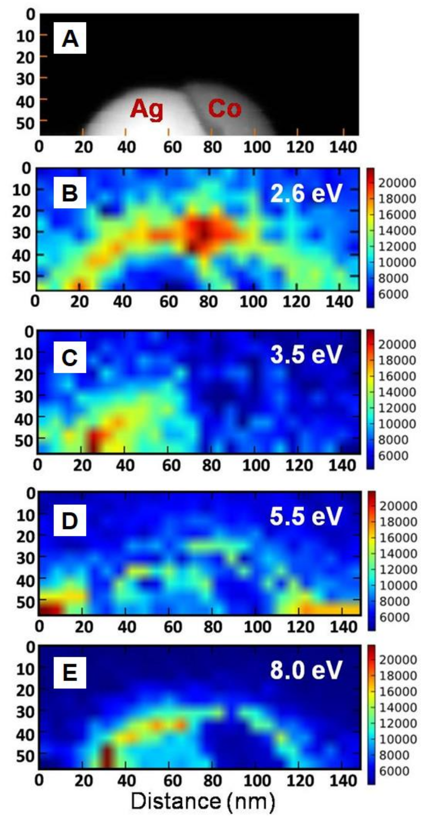

FIGURE 2

Map of plasmon energies occurring on the surface and in the bulk of bimetal nanoparticles. EELS mapping at the surface and bulk positions in the bimetal nanoparticles was used to reveal the nature of spatial decay, energy, and intensity of the various plasmons.[6] The visible energy ferroplasmon is clearly evident in (**B**) as intense signals at the interface of the Ag-Co as well as on the surface of Co.

B. Identification and Manipulation of Novel Topological Phases

Professor N. Gedik, MIT, Single Investigator

Topological insulators are materials that are electrically insulating in the bulk yet possess a band structure which requires that the surface conduct. The theoretical prediction and subsequent discovery of topological insulators several years ago ushered in a new era for this materials family in which novel physics is readily evident. The original discovery revealed that the conducting surface states are equivalent to spin-locked forms of the quantum Hall state – without the need for ultralow temperatures or high magnetic fields. Though materials challenges have prevented the physics from being expressed at ambient conditions thus far, studies in this field have resulted in a wide family of unique electronic states that do not result from symmetry breaking.

The topological surface states of a prototypical topological insulator, Bi_2Se_3, lie within the bulk bandgap of the material and, as a result, it is a relatively ideal material system in which to optically manipulate electronic states. By carefully choosing the energy of such an optical pulse, one can avoid exciting electrons or holes from the bulk and minimize exciton formation and electron-phonon interactions which may obscure more interesting phenomena.

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[6] Passarelli N, Perez LA, and Coronado EA. (2014). Plasmonic Interactions: From Molecular Plasmonics and Fano Resonances to Ferroplasmons. *ACS Nano*. 8:9723-9728.

A particularly intriguing approach to manipulating electronic states in the solid state is to consider Floquet physics. The Floquet theorem actually predates the Bloch equation and mathematically the two are intimately related. More specifically, Floquet physics is manifestation of a time-domain equivalent of the Bloch theorem and shows that the time-periodic potential of an applied electromagnetic field can induce new electronic states. The energetically isolated topological surface states of Bi_2Se_3 are ideally suited to search for such induced states.

To study the electronic states of Bi_2Se_3, Professor Gedik employed angle resolved photoemission spectroscopy (ARPES). This energy- and momentum-resolved technique allows the direct observation of the electronic structure of a material and clearly reveals the topological surface states. To study the Floquet physics in this system, he employed a time-resolved version of ARPES during and after the impinging of a mid-infrared laser pulse on the sample (see FIGURE 3).

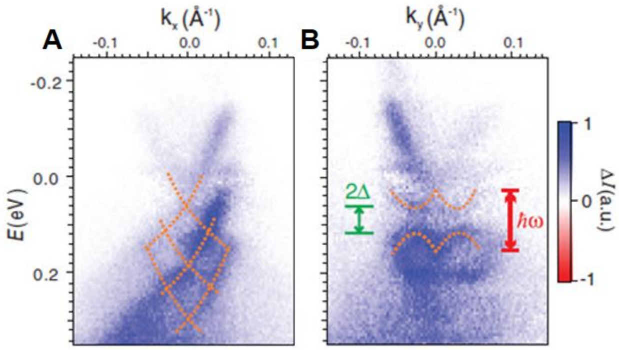

FIGURE 3

Exploring Floquet physics in Bi2Se3 using ARPES. The panels show ARPES spectra collected (**A**) during and (**B**) after a linearly polarized infrared pulse was impinging the sample (the unperturbed spectra have been subtracted out for clarity). Spectra are shown through Γ along the k_x (parallel to the applied electric field) and k_y (perpendicular to the applied field) directions. As discussed in the text, one can see "copies" of the electronic structure at energies offset by integer numbers of the infrared photon energy. Additionally, and consistent with theory, one can see Floquet-Bloch bands open band gaps along k_y. The dashed orange lines are a visual guide.

As expected from theoretical predictions, the infrared light induces "copies" of the Bi_2Se_3 electronic structure at energies offset by integer numbers of the infrared photon energy both above and below the non-illuminated electronic structure. Furthermore, these states interact or hybridize according to selection rules and either open gaps or retain band crossings. In the event of using circularly polarized light, the work shown here breaks time-reversal symmetry with an electromagnetic field inducing band gaps and thus optically turns off the topological surface states. This breaking of time-reversal symmetry with an electromagnetic field represents a completely different approach to engineering novel states of matter on the surface of a topological insulator.

The observation of Floquet physics in a three dimensional topological insulator represents the first such observation in a solid material and these experiments ultimately pave the way for using lasers to engineer novel photon-dressed states with readily synthesized materials. Additionally, the results indicate a manifestation of the long sought-after quantum Hall phase without Landau levels, the observation of which provides an important step towards photon-induced Floquet Majorana modes and the possibility of optically-controlled topological quantum computation.

C. Unique Electronic Transport Physics in a 3D Analog of Graphene

Professor R. J. Cava, Princeton University, MURI Award

Graphene has attracted a great deal of attention since its isolation in 2004 for its striking mechanical and electronic properties. For example, it possesses electrons that effectively travel as massless particles near the speed of light. Graphene's remarkable electron mobility stems from the fact that the massless Dirac equation typical to particle physics governs its transport properties rather than the Schrödinger equation typical to condensed matter. The band structure reveals that, unlike a metal with overlapping valance and conduction bands or even a traditional semimetal with slightly overlapping bands, graphene supports a structure where the valance and conduction bands touch only at discrete points in momentum space called Dirac points. The dispersion moving away from these points is linear, and is called a Dirac semimetal (DSM) structure.

Graphene is a two dimensional (2D) material and the 2D Dirac fermions which give rise to its properties are common to another set of extraordinary materials: time-reversal invariant topological insulators. Thus, a logical question to ask is if three dimensional (3D) counterparts with equally unusual topologies and equally impressive properties exist. In FY14 that question was answered in the affirmative as multiple experimental groups, including Cava's, reported success in the hunt for a three dimensional Dirac semimetal (3D DSM). Previous theoretical work revealed that a 3D DSM could be obtained by tuning the interface between a topological insulator and a normal insulator under certain circumstances, but the Dirac points that arise in that case are accidental. A more robust approach is to use a material in which the predicted Dirac points are protected by crystalline symmetry. Cava and his team used one such material in their work, Cd_3As_2, and verified that it is a 3D DSM with angle resolved photoemission spectroscopy.

3D DSMs are interesting not only for their inherent properties, but also because they are theorized to be parent materials for systems that generate a plethora of novel physics. In particular, if either time-reversal or inversion symmetry is broken (but not both), 3D DSMs are expected to evolve into Weyl semimetals via a separation of the Dirac points in momentum space. Weyl nodes are topological objects which are robust against external perturbations and are predicted to harbor exotic effects such as Fermi arc surface states and chiral anomalous magnetotransport. As Cava's group extended their Cd_3As_2 studies to begin to explore such phenomena, they also uncovered physics unanticipated by prior theoretical work.

The unanticipated result arose in transport data that revealed a remarkable protection mechanism strongly suppressing backscattering in Cd_3As_2 samples in the absence of an applied magnetic field. The level of suppression fluctuates on a case by case basis, but under the protection, single crystal samples can exhibit mobilities as large as 9×10^6 $cm^2V^{-1}s^{-1}$ at 5 K. This astonishing number places these mobilities in an ultrahigh regime populated by materials such as high purity bismuth. The protection mechanism is destroyed, however, when a magnetic field is applied and a very large magnetoresistance (MR) results. This MR is observed in all samples, but its character does differ slightly depending on the sample under observation and the strength and direction of the applied field. An example of the MR behavior in a crystalline sample with a high mobility is shown in FIGURE 4. While this high field power law behavior is only seen in some samples with high mobility, the linear behavior is present at all field strengths in single crystal low mobility and multi-domain samples. This linear behavior is rare in metals and semimetals but it has been observed in two topological insulators. Additionally, and as shown in the figure, the MR depends on the angle of the applied field with respect to the crystal structure of the sample. While the group has hypothesized that these behaviors may relate to changes in the Fermi surface induced by the applied field, the physics is not understood at this time.

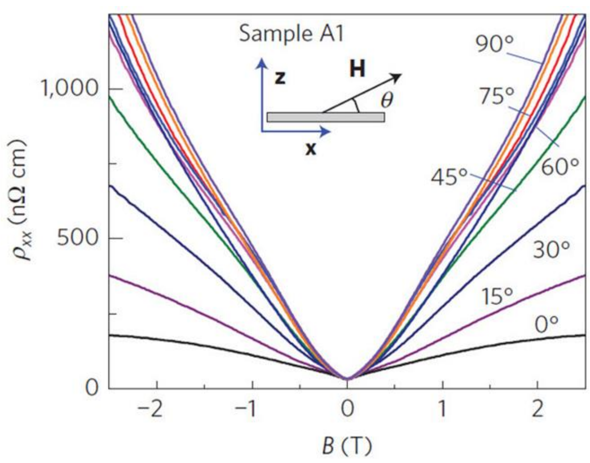

FIGURE 4

The resistivity of a single crystalline, high mobility 3D DSM Cd_3As_2 sample is shown as a function of applied magnetic field. At low field values (~0-2 T) the MR is nearly linear in applied field, H (where $B = \mu_0 H$), while at higher fields the MR follows an H^α power law. Values for α vary by sample, but the sample shown here an α of 2.55. As the angle of the applied field changes in the x-z plane the MR also changes and becomes negative for θ values less than 5^0.

The Cava group extracted further information about the Cd_3As_2 band structure from Landau level spectroscopy measurements. This data showed that the linear dispersion and high Fermi velocity of Cd_3As_2's electrons extend beyond the anticipated energy limits for the behavior. This effect, which cannot be considered as the limit of normal band structures, could be critical to understanding the high mobilities and large magnetoresistance observed in the transport measurements.

Additional work by the group following the spectroscopy experiments produced a model band structure consistent with the experimental findings and suggests that Weyl fermions are in fact the low-energy excitations in Cd_3As_2, but additional studies are needed before any full understanding is complete. This work must extend to the theorists as well as recent experimental results such as Cava's illustrate that the current theoretical framework does not allow a full description of the observed phenomena in topological 3D DSMs.

D. Magneto-optical Trapping of a Diatomic Molecule

Professor David DeMille, Yale University, MURI and Single Investigator Awards

Professor DeMille's research group is investigating methods for laser cooling and trapping molecules. The ultimate goal of this research is to develop direct methods of cooling and trapping molecules to take advantage of their non-symmetric long range interactions. In FY14, Professor DeMille's research team reported the first demonstration of a three-dimensional magneto-optical trapping of the diatomic molecule, strontium monoflouride (SrF), at a temperature of approximately 2.5 millikelvin, the lowest yet achieved by direct cooling of a molecule.[7] The direct cooling and trapping of molecules is an important achievement that impacts several scientific applications ranging from precision measurement, quantum simulation, quantum information to ultracold quantum chemistry (see FIGURE 5).

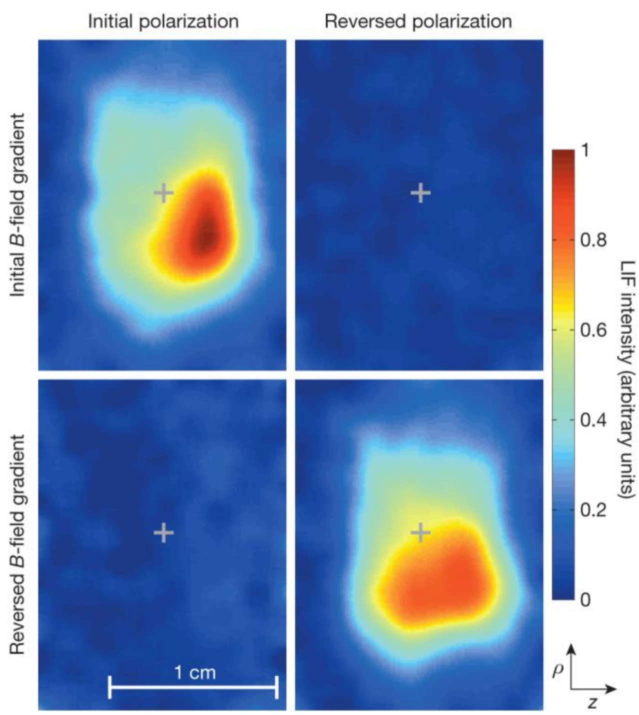

FIGURE 5

Magneto-optical trapping of SrF. The panels reveal light induced fluorescence in the trapping region for different polarizations and signs of the magnetic field gradient reveals the cloud of trapped SrF molecules

[7] J.F. Barry, D. J. McCarron, E. B. Norrgard, M. H. Stenecker, & D. DeMille (2014) Magneto-optical trapping of a diatomic molecule. *Nature* 512:286-289.

Several creative methods are being explored to overcome the technical challenges of cooling molecules in an effort to exploit their rich internal structure and non-isotropic interactions. Studying this rich structure reveals important insights in quantum chemistry, novel methods suitable for quantum information, exploration of exotic states of matter such as chiral spin liquids, and improved tests for fundamental violations and variations. These rich potential features that are the result of complex internal structure also makes molecules more difficult to laser cool and trap compared to neutral atoms. It is desirable to prepare the molecules in the rovibrational ground state. These states are not governed by strict selection rules. Additionally, traditional collisional, or sympathetic, cooling methods are inefficient at quenching molecular vibrational motion. The DeMille group has demonstrated a straightforward method for directly laser cooling and trapping SrF molecules. In addition, it is anticipated that the method should be applicable to a large range of other molecular species.

E. Multi-Qubit Enhanced Sensing and Metrology

Professor Paola Cappellaro, MIT, MURI Award

The ability to protect systems of multiple qubits from decoherence is crucial in the effort to enhance the sensitivity of quantum sensors. In FY14, the MURI team led by Professor Cappellaro demonstrated that spin decoherence times in nitrogen vacancy (NV) sensor systems can be dramatically improved by using a technique called dynamic decoupling. The advantages of this technique are not limited to decoherence issues, however, and generalized versions of it can be used to extract information about the fields of many samples of interest. While multiple difficulties exist in developing a full reconstruction of time dependent fields with a single quantum probe, combating these difficulties was made easier this year by a key insight from the group: coherent manipulations of the sensor can simultaneously decouple it from sources of decoherence and create filters that extract information about field dynamics. While this realization opens the door to advancing applications such as nano-scale imaging of nuclear spins, one also needs enhanced spatial resolution to develop a full picture of complex structures. A method proposed this year for a NV sensor system provides exactly this enhancement and brings the sensor's spatial resolution down to atomic scales. In total, the work provides a protocol that allows the sensing of individual nuclear spins and their mutual couplings with atomic-scale spatial resolution. This combination allows one to extract a wealth of information about local characteristics of complex molecular structures, such as a biological system (see FIGURE 6).

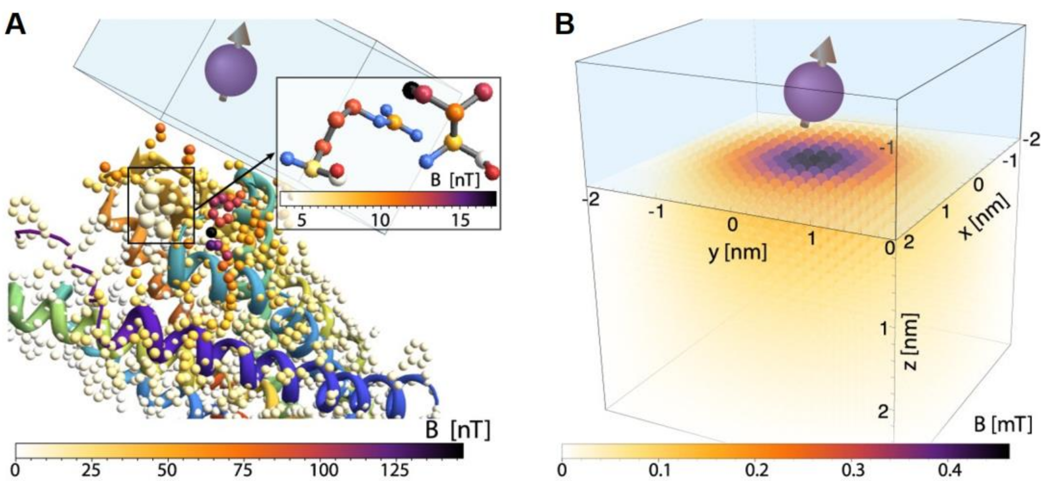

FIGURE 6

Dynamic decoupling to improve spin decoherence times in NV sensor systems, as illustrated in a biological system. (**A**) Nuclear spin imaging with a shallow NV center in diamond. A single NV spin (purple) at 1-2 nm from the diamond surface can sense single nuclear spins in a molecule (the chemokine receptor CXCR4, (ribbon diagram) anchored to the diamond. The magnetic field produced by individual ^{13}C (spheres with color scale given by the coupling strength) is in the range of nT, within reach of NV sensitivity. Inset: the binding site of interest (atoms other than ^{13}C are blue, O, and red, N). (**B**) A shallow NV center (2 nm from the surface) creates a magnetic field gradient above the [111] surface of the diamond. Note the azimuthal symmetry of the field, which causes degeneracy of the frequency shift at many spatial locations.

F. Quantum Computing, Quantum Control, and Quantized Nonlinear Optics with Superconducting Circuits

Professor Andrew Houck, Princeton University, PECASE Award

Simulating quantum phenomena on classical computers often quickly becomes an intractable task. The field of quantum simulation aims to remove the classical component of the solution and employ a controlled quantum mechanical device to investigate more complicated quantum systems. Superconducting cavity lattices present one option for realizing one of these "quantum simulators."

Professor Houck's team has made exciting progress toward developing a tool to provide local site information for such lattices to characterize them (see FIGURE 7). The work monitors the transmission through the array while scanning a small piece of dielectric above the lattice, locally inserting a lattice defect. By monitoring the change in transmission as function of defect position one can infer the strength of the normal mode weight at the probed lattice site. This process is similar to scanned gate microscopy in 2-d electron gas measurements, but with photons. This technique can be used to reconstruct normal mode maps and to date the agreement between experimentally observed and theoretically predicted mode maps is excellent. When qubits are added to the system it could produce a microscopy technique with single lattice site resolution akin to the quantum gas microscope for cold atoms. The ongoing characterization work will be essential in ultimately verifying behaviors observed in these lattices during the study quantum phase transitions.

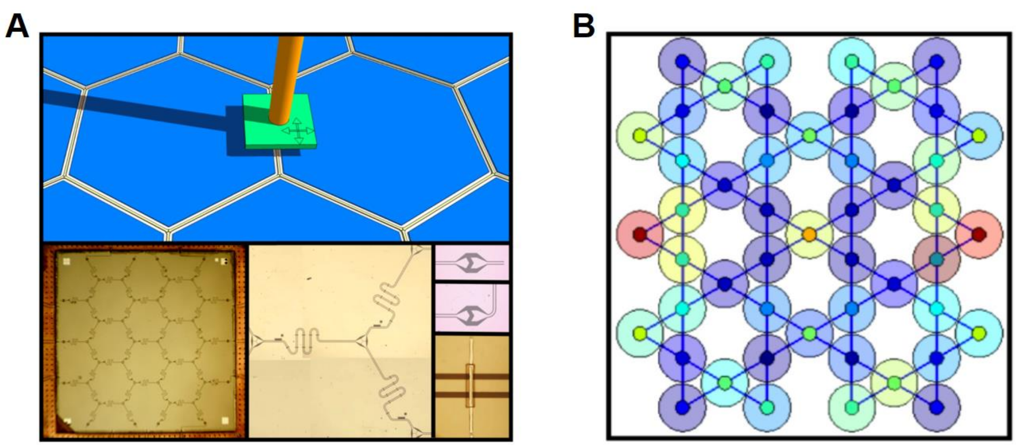

FIGURE 7

Scanned defect microscopy of a superconducting cavity lattice. A sapphire dielectric (**A**, top) is scanned above a 50-cavity lattice (**A**, bottom). Monitoring change in transmission at any given mode allows reconstruction of that normal mode. Experimentally-extracted values (**B**, outer circles) agreed with theoretical predictions (**B**, inner circles).

G. Cavity QED and Devices Based on Quantum Dot Molecules in Optical Nanocavities

Professor Jelena Vuckovic, Stanford University, Single Investigator Award

Quantum dot molecules have a rich structure of energy levels which can be electrically tuned over a wide range. The ability to embed such electrically tunable multi-level quantum systems inside optical cavities opens many avenues for exploration including both fundamental studies and novel applications. One such application is the ability to successfully generate nonclassical light. Nonclassical light states on chips are of particular interest as they will be needed for future optical quantum hardware. It is well known that strongly coupled quantum dot-photonic crystal cavity systems exhibit optical nonlinearities at the single photon level and can be used to generate such nonclassical light. Experimental investigation of the effect, however, has focused only on cases in which the dot is on or near resonance with the cavity.

In FY14, Professor Vuckovic's group departed from this convention and used a highly detuned system to demonstrate an effect (photon-blockade) which can be used to generate nonclassical light. Not only do the results show that the generation of nearly perfect single photon streams is possible in this detuned configuration, but they additionally illustrate the key role that detuning plays in the high-fidelity generation of indistinguishable photons (see FIGURE 8). As a whole, this work reveals detuning is a key-ingredient for high-fidelity on-chip generation of indistinguishable photons, and also paves the way for additional exploration of theoretical proposals operating in the far-detuned regime.

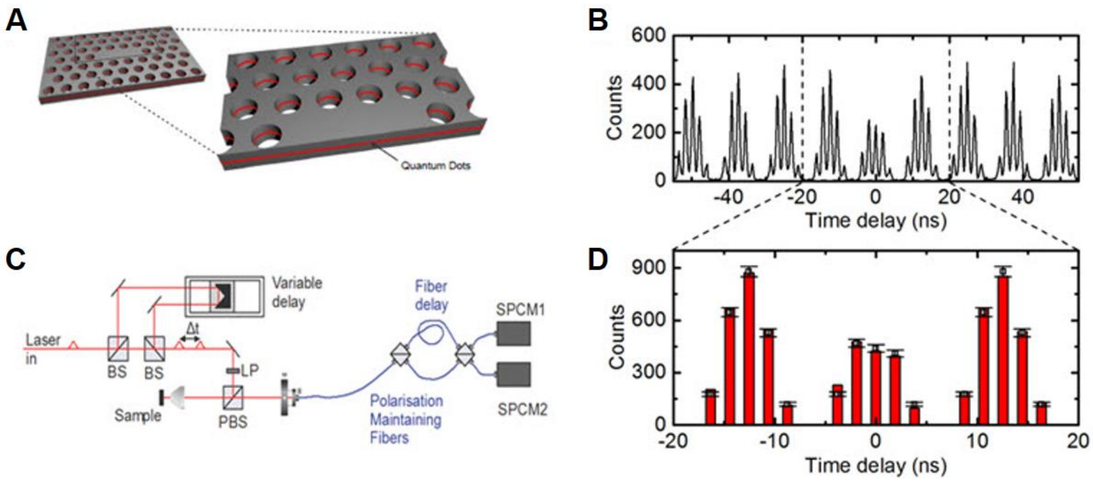

FIGURE 8

Role of detuning in high-fidelity generation of indistinguishable photons. (A) Schematic illustration of a self-assembled quantum dot embedded in a photonic crystal cavity. (B) Schematic illustration of the setup used to measure photon indistinguishability. (C) Measured correlation function of the transmitted photon stream showing five peaks per excitation pulse pair, corresponding to various combinations of paths of the 2 photons from the pair through the HOM interferometer. At 0 time delay the amplitude of the three center peaks is reduced. (D) Amplitudes around zero delay obtained from binning the data presented in (c) with a temporal width of 512ps about the center of each peak. Fits to the data are presented as black data points and reveal $g^2(0)=0.5$ and an indistinguishability of V=0.6.

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 to external organizations and customers.

A. Structured Light Imaging Through Obscurants and the Vein Eye Camera

Investigator: Professor Robert Alfano, City University of New York, HBCU/MI and REP Awards
Recipient: Industry

The objective of Professor Alfano's ARO-funded work is to explore the polarization effects of Laguerre-Gaussian modes as they propagate through various media, providing insight in how to control light transmission through various obscurants. His laboratory examined a geometric phase arising from transformations along the surface of a Poincare sphere representation for cylindrical vector beams. Cylindrical vector beams are expressed as the superposition of orthogonal circular polarized Laguerre-Gaussian modes of opposite topological charge. Two spheres are described where the poles of each sphere are circular polarized Laguerre-Gaussian modes, and points along the equator are cylindrical vector beams. A closed loop transformation on the sphere's surface is carried out using combinations of wave plates and cylindrical lens mode converters, and an acquired geometric phase is experimentally measured via interferometry.

The results of these studies led to an unexpected transition based on new insights into polarization-changing interactions with turbid media, photon propagation, and how scattering and absorption can change in various biological systems, such as veins or tumors in a human body. This research, in collaboration with the University of California and Lawrence Livermore National Laboratory, directly led to transitions to industry for the development of devices which use light to detect breast and prostate cancer as well as allow imaging through adverse atmospheric conditions. The Vein-Eye Camera, which uses two salient properties of light – polarization and near infrared wavelengths, was developed to visualize veins under skin layer. It is now being marketed as a rapid, non-invasive method to detect veins and monitor blood flow.

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. The Behavior of Electrons in Materials with both Strong Correlations and Spin-Orbit Coupling

Professor David Hsieh, California Institute of Technology, Single Investigator Award

Spin-orbit coupling has emerged as a major theme within condensed matter physics, due to the important role it played in the emergence of topological insulators. A particularly important area of investigation is the physics of electrons, among other things, in the presence of both spin-orbit coupling and strong correlations. The intersection of these two regimes is anticipated to reveal new scientific and future technological opportunities. A key technique for the investigation of the physics of electrons in solids is non-linear optical techniques. These techniques reveal aspects of band structure, conductivity and crystal symmetry. They are particularly useful in revealing underlying physics and materials properties without the complications of making physical contact with the sample. However, a key element is typically missing in these techniques: spatial resolution. Important phenomena often involve, for example, a spatially non-uniform phase transition. Though able to distinguish separate phases, non-linear optics without spatial resolution will not be able to observe a transition clearly nor distinguish the physics active in the separate phases. Dr. Hsieh is developing techniques that will add spatial resolution – imaging – to several traditional non-linear optical spectroscopies to overcome this difficulty. As a result, new insights into strongly correlated materials with significant spin-orbit coupling are expected.

B. Quantum Limited Electrometry and Ultra-Strong Photon-Phonon Coupling Using a Cavity-Embedded Single Cooper Pair Transistor

Professor Alexander Rimberg, Dartmouth College, Single Investigator Award

This project leverages advancements in the ability to probe and control the quantum state of electrical and mechanical devices in order to study more general quantum systems. In particular, the research uses the circuit quantum electrodynamics (cQED) architecture in which superconducting devices such as Cooper pair transistors (CPTs), are placed inside high Q microwave cavities to allow for ultra-sensitive and, in principle, quantum-limited charge detection. To demonstrate the power of this technique, the group will couple the cavity embedded CTPs to nanomechanical resonators with the goal of using the CPTs to monitor the resonator positions. Apart from the intrinsic interest of the systems, resonators such as these have numerous potential applications such as force and mass sensing and in the future they may provide couplings between optical and microwave quantum systems. During the first year of support for this project multiple hardware systems were configured and significant progress was achieved in sample fabrication and measurement technique development. It is anticipated that in FY16 these individual components will be integrated into a functioning whole to begin data collection.

C. Quantum Computing, Control, and Quantized Nonlinear Optics with Superconducting Circuits

Professor Andrew Houck, Princeton University, PECASE Award

Simulating quantum phenomena on classical computers often quickly becomes an intractable task. This research aims to remove the classical component of the solution and employ a controlled quantum mechanical device to investigate more complicated quantum systems. Superconducting cavity lattices present one option for realizing one of these "quantum simulators."

Professor Houck's team has made exciting progress toward developing a tool to provide local site information for such lattices to characterize them, as noted in Section III-F. It is anticipated that in FY15, qubits will be added to cavity lattices. This will enable the study of non-linearities and the ability to look for signatures of photonic quantum phase transitions. A multimodal structure will be created by building a very low frequency superconducting cavity with a small free spectral range operating at a high mode number in the cavity. If one obtains a large qubit-cavity coupling in comparison to the free spectral range, effective interactions between photons in different modes are introduced. In the following year the researchers will characterize multi-mode emission from this system and look at the generation of photons at all modes when only one is driven in a process that may produce quantum (nonclassical) or even entangled photons.

D. Light Filamentation

Professors Natalia Litchinitser, SUNY - Buffalo, and Martin Richardson, University of Central Florida, MURI Award

One of the fundamental challenges in transmitting and routing microwaves in air is inevitable divergence because of diffraction, and the lack of guiding and beam steering “components” when the beam propagates in free space. Moreover, detection of radar signals in a realistic environment may be negatively affected by the divergence of the beam resulting from distortions by natural obstacles, e.g., by non-planar landscapes. To overcome the distortion of beams propagating in such environments, some way of guiding the beam around obstacles is necessary.

The development of ordered structures of laser-induced plasma filaments opens the possibility of creating conductive filamentary structures capable of guiding microwave frequency beams. In the last few years, various types of filament-based waveguides have been proposed for channeling microwaves. While this approach offers a way to counteract the diffraction of a radar signal over some distance, the issues of beam steering and coupling microwave signals into such waveguides are likely to be challenging.

The goal of this project is to test a fundamentally-new approach based on unique physical properties of virtual hyperbolic metamaterials (vHMM) formed of plasma filaments in air. The research team has modeled these structures, with results suggesting that they are capable of focusing, guiding and steering signals to facilitate new degrees of freedom in the detection of such signals in realistic environments (see FIGURE 9). Conventionally, hyperbolic metamaterials are realized using either metal/dielectric multilayers or an array of metal wires in a dielectric matrix.

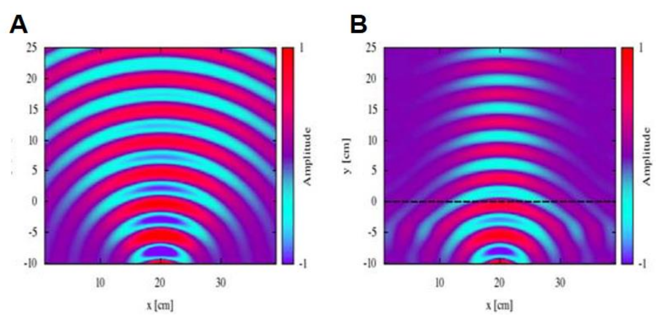

FIGURE 9

The field intensity distribution for TM-polarized continuous wave Gaussian beam at wavelength λ=5 cm propagating in (A) air and (B) in a virtual hyperbolic metamaterial.

The team has simulated an array of plasma filaments formed by the propagation of intense short pulses in air and demonstrated the theoretical formation of a virtual hyperbolic metamaterial structure. Indeed, plasma filaments play the role of metal wires and the air plays the role of a dielectric host. It is anticipated that the research team will validate these results experimentally in FY15.

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