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14. ABSTRACT A symposium was organized at the national meeting of the American Chemical Society in Boston, MA (August 16-20, 2015). The session highlighted cutting-edge research efforts across several disciplines that focused on building a fundamental understanding of surface chemistry involving real catalysts under ambient conditions of temperature and pressure. This symposium brought together approximately 20 researchers and graduate students from around the world whose work impacts this important field. Fruitful discussions, based on presentations, helped to educate the attendees, seed them with new ideas, and motivate new research in this area of importance to the Army and					
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Report Title

Final Report: 250th National ACS Meeting Symposium Entitled: Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions

ABSTRACT

A symposium was organized at the national meeting of the American Chemical Society in Boston, MA (August 16-20, 2015). The session highlighted cutting-edge research efforts across several disciplines that focused on building a fundamental understanding of surface chemistry involving real catalysts under ambient conditions of temperature and pressure. This symposium brought together approximately 20 researchers and graduate students from around the world whose work impacts this important field. Fruitful discussions, based on presentations, helped to educate the attendees, seed them with new ideas, and motivate new research in this area of importance to the Army and greater society.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received

Paper

TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received

Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Christopher Karwacki	0.00	
FTE Equivalent:	0.00	
Total Number:	1	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See Attachment

Technology Transfer

Final Report

(W911NF-15-1-0186)

Symposium on “Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts under Ambient Conditions” at the 250th ACS National Meeting in Boston, MA

John R. Morris, Virginia Tech

Overview

The primary objective of this work was to organize and conduct a symposium at the national meeting of the American Chemical Society in Boston, MA (August 16-20, 2015). The session highlighted cutting-edge research efforts across several disciplines that focused on building a fundamental understanding of surface chemistry involving real catalysts under ambient conditions of temperature and pressure. This symposium was a tremendous success and brought together approximately 20 researchers and graduate students from around the world whose work impacts this important field.

Relation of the Symposium to the ARO Research Interests

Operando spectroscopy and surface chemistry, including catalytic and sensor chemistry, provide critical foundations for numerous practical material-based applications essential to the ARMY, DOD and the larger society. The field is relatively new and rapidly emerging as one of the most interdisciplinary with active collaborations between synthetic material chemists, experimental surface scientists, and theorists.

The symposium provided an important forum to discuss the most challenging aspects of operando based techniques, such as the ability to effectively integrate experimental measurements and theoretical predictions into a single framework. The breadth of topics covered and the depth of originality and innovation of the speakers provided attendees with new knowledge and ideas from multiple perspectives and experiences for advancing the field. The topics discussed at the symposium addressed, from a fundamental point of view, many key practical areas of concern to the Army relevant to soldier protection, future combat systems, and enhancing soldier performance. The topics also advanced the DOD strategic research areas of nanoscience and nanotechnology.

The symposium covered a wide range of topics in surface and colloid science, as reflected by the research interests and reputations of the invited speakers (see below). While the topics did not ignore the well established themes of colloid and surface science, the focus was on emerging areas such as operando based and related computational techniques that emphasize structure-activity information for the design of functional materials. Specific areas discussed during the symposium included: novel advanced in-situ experimental techniques, interfacial binding and diffusion of molecules on catalyst surfaces, techniques that characterize changes in the structural order of active phases, techniques that correlate surface reactions with structural properties, *ab initio* DFT and molecular dynamic simulations of self-assembled systems, and the role of defect and disordered states in complex catalysts. Abstracts of presentations are available online at the ACS meeting website.

In addition to the successful communication and dissemination of scientific discoveries, the symposium provided numerous opportunities for researchers to uncover new areas for potential research directions as well as a forum for new collaborations in the areas highlighted above.

Invited Scientists: *Several of the Top Researchers in the World Contributed*

The speakers for the special symposium were invited based on their established reputations in the field of colloid and surface science. They are leading researchers in the broad scientific community of colloid and surface science, specializing in numerous topics of fundamental and applied importance. In addition to the invited speakers, a number of contributed oral presentations were selected. A complete list of presentations for this symposium can be found at the ACS Meeting Website (see <http://boston2015onsite.acs.org/t/173565-ac-s-national-meeting-boston-2015>).

Invitee	Affiliation
Anatoly Frenkel	Yeshiva University, New York
Israel Wachs	Lehigh University
Miquel Salmeron	Lawrence Berkeley National Laboratory
Hendrik Bluhm	Lawrence Berkeley National Laboratory
Jinghua Guo	Lawrence Berkeley National Laboratory
David Starr	Helmholtz-Zentrum Berlin für Materialien und Energie
Ethan Crumlin	Lawrence Berkeley National Laboratory
Mark Newton	The European Synchrotron Radiation Facility, France
Peter Chupas	Argonne National Laboratory
Karena Chapman	Argonne National Laboratory
Jeff Miller	Argonne National Laboratory
Trudy Bolin	Argonne National Laboratory
Jose A. Rodriguez	Brookhaven National Laboratory
Franklin Tao	University of Notre Dame
Sanjaya Senanayake	Brookhaven National Laboratory