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RPPR Final Report
as of 03-Jan-2019

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STEM Degrees: **STEM Participants:**

Major Goals: The objective of this project was to organize a symposium at the Fall 2017 National Meeting of the American Chemical Society with a focus on developing a fundamental understanding of catalytic chemistry facilitated by metal-organic frameworks (MOFs). Specifically, this symposium presented recent advances in our fundamental understanding of chemical reactions and dynamics within a variety of MOFs using both experimental and theoretical approaches. The overarching goal of the symposium was to provide an overview of the state-of-the-art in MOF-based catalysts, with particular emphasis on energy-related applications, environmental sciences, and industrial chemical production. Interplay between measurements and simulations was a key role in the discussions.

Accomplishments: This symposium successfully brought together approximately 20 researchers and graduate students from across the country whose work impacts the general field of catalysis with a special focus on MOFs. Presentations and discussions were encouraged to focus specifically at building rules for predicting the outcome of various molecule-MOF interactions. Importantly, this effort has helped to produce a better understanding of issues of practical importance, including (but not limited to) toxic chemical decontamination, sensor development, molecular separations, and the environmental remediation of toxic molecules.

Training Opportunities: The average number of graduate students who attended the lectures is estimated to be 20 and another 10 students presented work at the symposium. In addition, approximately 7 postdoctoral associates attended the symposium. The symposium exposed these scientists to a wide variety of topics and served as an excellent training ground for the next generation of researchers in this field. In addition to the lectures, students learned from small group discussions that emerged following each session.

Results Dissemination: The abstracts from each presentation have been archived at the American Chemical Society and are available to the general public through several types of database searches including ISI Web of Knowledge. Those abstracts provide the name of each presenter, whom the interested party may contact for further information regarding the topic.

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

RPPR Final Report
as of 03-Jan-2019

PARTICIPANTS:

Participant Type: PD/PI
Participant: John R. Morris
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Co-Investigator
Participant: Amanda J. Morris
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
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Other Collaborators:

Symposium at the 254th American Chemical Society National Meeting: Fundamentals of Metal Organic Framework Catalysis

John R. Morris, Virginia Tech

Abstract. The ACS symposium advanced the general field of catalysis with a focus on fundamental studies of new metal-organic frameworks (MOFs). Metal organic frameworks offer the potential of molecular-based catalysts that can be tailored at the atomic level to achieve efficient turnover and high performance. This topic is of critical importance and is broad enough to reach many communities within the catalysis field, including enantioselective catalysis, environmental remediation, detoxification of chemical warfare agents, and artificial photosynthetic chemistry. This symposium successfully brought together these complementary fields to facilitate idea-sharing and scientific collaboration.

Overview. The symposium covered a wide range of topics in metal-organic framework chemistry and catalysis, as reflected by the research interests and international renown of all the invited speakers. While the topics did not ignore the well-established themes of metal-organic frameworks, the focus was on emerging areas such as energy conversion and related computational techniques that emphasized structure-activity information for the design of functional materials.

Some of the topical areas covered at this symposium included the following: novel advanced *in-situ* experimental techniques, interfacial binding and diffusion of molecules on catalyst frameworks, techniques that characterize changes in the structural order of active phases, techniques that correlate 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, and coupling experimental and computational information.

Army Relevance. This symposium brought together experts in many areas of research ranging from catalysis on surfaces to adsorption and reactions on organic films and chemistry on environmental surfaces. The type of scientific advances that can emerge from a meeting of this nature is central to the ARO's mission of enhancing the Army's capabilities through research. By working to develop rules that help scientists better predict the outcome of molecule-surface interactions, the promulgation of the latest advances in this broad field will aid in the rational design of catalysts, protective coatings and paints, and filter technology—all of which will have a positive impact on protecting soldiers on the battlefield.

Scientists and Presentation Titles. The speakers for this special symposium were personally invited based on their established reputations in the field of MOF-based catalysis. They are the leading researchers in the broad scientific community of catalysis, specializing in numerous topics of fundamental and applied importance. The speakers who participated in the symposium are listed below.

Presentation Title	Presenter
Robust surface-anchored UiO-66-based metal-organic-framework films on polymer fibers for rapid hydrolysis of chemical agents	Gregory Parsons
Metal organic framework's acid dissociation constants as a robust descriptor of their morphology and reactivity: Applications to hydrolysis of warfare agents	Mohammad R. Momeni
Reaction of the Chemical Warfare Agent Simulant, DMMP(g), with Zirconium (IV) MOFs: An Ultrahigh-vacuum and DFT Study	Guanyu Wang
Molecular modeling insights into the adsorption and degradation of hazardous chemical warfare agents by metal-organic frameworks	Jacob Harvey
Optimizing toxic chemical removal through defect-induced UiO-66-NH2 metal-organic framework	Greg Peterson
Insights into the MOF-based Degradation of Organophosphates in Non-Aqueous Media: a Combined Experimental-Modeling Study	Dorina Sava Gallis
Uptake and diffusion of chemical warfare agent simulants in Zr6-based MOFs	Conor Sharp
Metal–Organic frameworks as highly functional catalytic arrays	Omar Farha
Modeling reactions catalyzed by noble metal clusters deposited on metal-organic frameworks	Andreas Mavrandonakis
Tandem Catalysis by Metal@MOFs with extremely high selectivity	Wenyu Huang
Controlled encapsulation of catalysts into nanoporous materials	Chia-Kuang Tsung
Nanospace within Metal-Organic Frameworks: Plenty of Opportunities for Heterogeneous Catalysis	Shengqian Ma
Computational study of A MOF-supported single site Ni catalyst for ethylene dimerization	Jingyun Ye
Single-Site Heterogeneous Catalysts for Olefin Upgrading Enabled by Cation Exchange in Metal-Organic Frameworks	Mircea Dinca
Inorganometallic catalyst design: Alkane metathesis catalysis in NU-1000 MOFs functionalized with transition metals	Bo Yang
Hydroxylation Stereochemistry as a Probe of In-MOF versus On-MOF Catalysis	David Powers
Functionalized metal organic frameworks for CO2 reduction	Karl Johnson
Mechanistic study on CO2 hydrogenation and photocatalytic reduction using metal-organic frameworks	Cheng Wang
Ni-Cyclam-Based Metal-Organic Frameworks for Electrochemical Reduction of CO2	Jie Zhu
Investigations of Water Oxidation by Catalysts Incorporated Metal-Organic Frameworks	Shaoyang Lin
Molecular Catalysis of Energy Relevance in Metal-Organic Frameworks	Sascha Ott
Probing Framework-Restricted Metal Axial Ligation and Spin State Patterns in Iron-Porphyrin-Based Metal–Organic Framework Catalysts	Jenny Lockard
Development of Highly Stable Metal-Organic Frameworks for Applications in Catalysis	Pavel Usov
Metal Dithiolene Frameworks with Tunable Physical and Chemical	Smaranda

Properties	Marinescu
Enhancement in Molecular Catalysis Through Redox Hopping Metal Organic Framework Scaffold	Amanda Morris
Photophysical properties of crystalline self-assembled porous materials: Contribution of interchromophoric interactions and environment	Pravas Deria
Tune the catalytic selectivity of core-shell metal-organic frameworks (MOFs) by changing the length of the linker in the shell	Hongcai Zhou
Multi-Component Metal−Organic Frameworks as Cooperative Bimetallic Catalysts	Shuai Yuan
CuPd Mixed-Metal MOFs Characterized by UHV-FTIRS and HR-XPS	Penghu Guo
Metal-organic frameworks as micromotors with tunable engines and brakes	Xiao Yu
Impact Of Metal Substitution On Stability And Adsorption Properties Of MOF-74	Krista Walton