

# 2023 AFOSR Molecular Dynamics and Theoretical Chemistry Program Review

Dr. Michael Berman | May 16-18, 2023 | Arlington, VA -hybrid

Basic Research Innovation Collaboration Center (BRICC)  
4100 N Fairfax Drive, Suite 450 | Arlington, VA 22203

## Agenda Day 1 | Tuesday, May 16, 2023

Time	Topic	Speaker
8:05	<b>In-person Check-in / Virtual Log-in</b>	
8:30	High Resolution Photoelectron Spectroscopy of Vibrationally Excited Anions	Daniel Neumark, UC Berkeley
9:05	Probing Charge-transfer Neutralization Reactions of Atmospheric Relevance using the Ion Storage Facility DESIREE	Richard Thomas, Stockholm University
9:40	Common Early Barriers in Surface and Cluster Ion Reaction with O <sub>2</sub>	Nicholas Shuman, AFRL
10:15	<b>BREAK</b>	
10:45	Chemistry in Merged Molecular Beams and in Merged Microjets	Andreas Osterwalder, EPFL
11:20	Understanding and Controlling Chemistry at Interfaces using Ion Soft Landing	Julia Laskin, Purdue University
11:55	Magnetic and Charge Order in Transition Metal Dichalcogenide Heterostructures	Kwabena Bediako, UC Berkeley
12:30	<b>LUNCH</b>	
1:45	The Critical Role of Electrical Polarization in Thermochemical Surface Catalysis	Yogesh Surendranath, MIT
2:20	On the Fundamentals of Interfacial Solvation: Molecular Imaging, Atomistic Simulations, and Statistical Mechanics Models	Yingjie Zhang, University of Illinois Urbana-Champaign
2:55	Electrical Double Layer Modulation of Organic Reactions at Electrode Interfaces	Jesse McDaniel, Georgia Tech
3:30	<b>BREAK</b>	
3:50	Safe, Energy-dense Ionic Liquid Fuels for Electrochemical Devices	Karthish Manthiram, Caltech
4:25	From Ionic Liquids to Deep Eutectics: New Frontiers in Green Propellants	Steve Chambreau, AFRL
5:00	<b>Adjourn for Dinner (not provided)</b>	

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## Agenda Day 2 | Wednesday, May 17, 2023

Time	Topic	Speaker
8:05	In-person Check-in / Virtual Log-in	
8:30	Trapped Hole Diffusion in Semiconductor Nanocrystals and Related Photochemical and Photophysical Processes	Gordana Dukovic, University of Colorado Boulder
9:05	Ballistic Excitons in 2D Superatomic Crystals	Milan Delor, Columbia University
9:40	Extending the Promise of Stochastic Methods to Catalysis via Machine Learning	Brenda Rubenstein, Brown University
10:15	BREAK	
10:45	Polariton Chemistry: Challenges and Prospects	Joel Yuen-Zhou, UCSD
11:20	Suppressed Reactivity via Cavity-induced Selective Vibrational Cooling	Blake Simpkins, NRL
11:55	Recent Advances in Correlated Quantum Chemistry in the Condensed Phase	Garnet Chan, Caltech
12:30	LUNCH	
1:45	Ongoing Advances in the Simulation of Room Temperature Ionic Liquid Interfaces	Gregory Voth, University of Chicago
2:20	Program Status Update	Berman, AFOSR
2:50	BREAK	
3:10	Poster Session	
5:00	Adjourn for Dinner (not provided)	

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## Agenda Day 3 | Thursday, May 18, 2023

Time	Topic	Speaker
8:05	In-person Check-in / Virtual Log-in	
8:30	Plasmonic Photocatalysis with Antenna-Reactor Nanoparticle Complexes	Naomi Halas, Rice University
9:05	Direct Observation of Infrared Energy Transfer Using Focused Electron Beams	Jon Camden, University of Notre Dame
9:40	Plasmonic Substrates Modify Dehydration Reactions via Vibrational Strong Coupling	Matthew Sheldon, Texas A&M
10:00	Photonic Electrochemistry	Franz Geiger, Northwestern
10:15	BREAK	
10:45	The Chiral Induced Spin Selectivity (CISS) effect- From Electron Transfer in Biology to Spintronics	Ron Naaman, Weizmann Institute
11:20	Probing Spin Polarized Electron Dynamics at Photocatalytic Interfaces Using Circularly Polarized XUV Light	Robert Baker, Ohio State University
11:55	Ab Initio Open Quantum Dynamics for Spin and Electron Relaxation in Solids	Yuan Ping, UCSC
12:30	LUNCH	
1:45	Review of the AFOSR MURI: Mechanistic Studies of Microdroplet Chemistry	Richard Zare, Stanford University
2:20	An Integrated Experimental and Theoretical Approach Toward Understanding Novel Reactivity, Structure and Chemical Gradients in Aqueous Microdroplets	Robert Continetti, UCSD
2:40	Molecular Interactions, Machine Learning, and the Quest of Realistic Molecular Simulations	Francesco Paesani, UCSD
3:15	BREAK	
3:35	Unraveling the Initial Steps of the Ignition Chemistry of the Hypergolic Ionic Liquid [EMIM][CBH] with Nitric Acid Exploiting Chirped Pulse Triggered Droplet Merging	Ralf Kaiser, University of Hawaii
4:00	Unsupervised Reaction Pathways Search for the Oxidation of Hypergolic Ionic Liquids	Rui Sun, University of Hawaii
5:00	MEETING ENDS	