

# 2022 AFOSR Molecular Dynamics and Theoretical Chemistry Program Review

Dr. Michael Berman | May 24-26, 2022 | Virtual

## Agenda Day 1 | Tuesday, May 24, 2022 (all times EDT)

Time	Topic	Speaker
10:20	Registration / Login	
10:50	Intro Remarks	Michael R. Berman AFOSR
11:00	Plasmonic Photocatalysis with Antenna-Reactor Nanoparticle Complexes	Naomi Halas Rice University
11:30	Energy Transfer in Strained Metal Nanostructures	Kenneth Knappenberger Pennsylvania State University
12:00	Dynamics of Layered (2D) Pseudo-Halide Perovskites	Michael Fayer Stanford University
12:30	BREAK	
1:45	Ultrafast Molecular Polariton Dynamics	Wei Xiong UC San Diego
2:15	Understanding the Interplay of Complex Molecules with Complex Cavities	Aaron Rury Wayne State University
2:45	Energy Cascade in Carbon Nanotube Polaritons	Martin Zanni University of Wisconsin-Madison
3:15	LUNCH	
3:45	Vibrational SFG Probe Electrode/Catalyst/Electrolyte Interface: Electrode Induction Effect and Mapping Field Profile by Stark Shift Ruler	Tianquan Lian Emory University
4:15	Electrochemistry, Electron Transfer and Chiral Induced Spin Selectivity	Joseph Subotnik University of Pennsylvania
4:45	Hydrogen and Gold: Isotope Effects and Nanoparticles, Shaken not Stirred	James Mayer Yale University
5:15	MEETING ADJOURN	

Agenda Day 2   Wednesday, May 25, 2022 (all times EDT)		
Time	Topic	Speaker
10:20	Registration / Login	
10:50	Intro Remarks	Michael R. Berman AFOSR
11:00	Applications Of Hybrid High Resolution Mass Spectrometry/Cryogenic Ion Spectroscopy to Thermochemistry and Kinetics	Mark Johnson Yale University
11:30	Femtosecond Time-Resolved Electron Ionization Mass Spectrometry	Marcos Dantus Michigan State University
12:00	Metal-Catalyzed Combustion Chemistry studied with Cluster Ion Spectroscopy	Michael Duncan University of Georgia
12:30	BREAK	
1:45	Progress towards Automated Force Field Generation Useful for Ionic Liquid-Based Propulsion Systems	Benjamin Prince AFRL/RV
2:15	Studies of Dynamic Materials in Extreme Environments	Steven Sibener University of Chicago
2:45	Fluxional Cluster Catalysts for Endothermic Cooling	Anastassia Alexandrova UCLA
3:15	LUNCH	
3:45	Program Status Update	Michael R. Berman AFOSR
4:15-6:00	POSTER SESSION	
6:00	MEETING ADJOURN	

### Agenda Day 3 | Thursday, May 26, 2022 (all times EDT)

Time	Topic	Speaker
10:20	<b>Registration / Login</b>	
10:50	Intro Remarks	Michael R. Berman AFOSR
11:00	Multiconfiguration Pair-Density Functional Theory for Molecular Qubits	Laura Gagliardi University of Chicago
11:30	Intersystem Crossing from Light to Heavy Elements	Xiaosong Li University of Washington
12:00	Ultrafast Ion Hopping and Correlations in Solid State Electrolytes	Scott Cushing Caltech
12:30	<b>BREAK</b>	
1:45	The Surface Science of MXenes	Dmitri Talapin University of Chicago
2:15	Molecular Access to the High Density Of States in Inorganic Nanocrystals Enabled by Covalent Conjugation	Ming Lee Tang University of Utah
2:45	Artificial Atoms, Molecules, and Solids: Multiple Functions and Emergent Properties	Colin Nuckolls Columbia University
3:15	<b>LUNCH</b>	
3:45	The Electric Field from a Single Ion and Ionic Layers Measured by Vibrational Spectroscopy	Jahan Dawlaty University of Southern California
4:15	How Do Bacteria Respond to Environmental Challenges? Perspectives from Membrane Transport Studied by Nonlinear Light Scattering	Hai-Lung Dai Temple University
4:45	MURI-ice: From Understanding Molecular Interactions to Controlling Ice Formation	Francesco Paesani UC San Diego
5:15	<b>MEETING ADJOURN</b>	