

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 (See list of presenters on the last page)	
6:00	MEETING ADJOURN	

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

Time	Topic	Speaker
10:20	Registration / Login	
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	BREAK	
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	LUNCH	
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	MEETING ADJOURN	

Poster Session Presenters

Last Name	First Name	Institution
Alayyoub	Bader	University of Pennsylvania
Anderson	Scott	University of Utah
Armentrout	Peter	University of Utah
Baker	Robert	Ohio State University
Bowen	Kit	Johns Hopkins University
Camden	Jon	University of Notre Dame
Cao	Tianyu	University of Pennsylvania
Chambreau	Steve	AFRL
Cronin	Steve	USC
DeBlase	Andrew	Spectral Energies, LLC/AFRL
Dukovic	Gordana	University of Colorado Boulder
Eaves	Joel	University of Colorado Boulder
Heaven	Michael	Emory University
Kim	Shinae	Iowa State University
Leone	Stephen	University of California Berkeley
Li	Tao	Yale University
McDaniel	Jesse	Georgia Tech
Neumark	Daniel	UC Berkeley
Pachter	Ruth	AFRL/RX
Rubenstein	Brenda	Brown University
Schneider	Stefan	AFRL/RQRP
Sheldon	Matthew	Texas A&M University
Sun	Rui	University of Hawaii
Sweeny	Brendan	Boston College ISR
Vura-Weis	Josh	University of Illinois at Urbana-Champaign
Wen	Xuelan	Princeton University
Yang	Nan	University of Wisconsin Madsion
Yuen-Zhou	Joel	UC San Diego
Zhang	Yingjie	University of Illinois at Urbana-Champaign