

2019 AFOSR Molecular Dynamics/Theoretical Chemistry Program Review

Dr. Michael Berman | May 21-23, 2019 | Washington, DC

U.S. Department of the Interior
1849 C Street, N.W. | Sidney Yates Auditorium
Washington, DC 20240

Agenda Day 1 | Tuesday, May 21, 2019

Time	Topic	Speaker
8:00	Registration	
8:30	Probing Element-Specific Charge Carrier Dynamics at Junctions	Stephen R. Leone UC Berkeley
9:05	Local Electric Fields at the Interfaces of Ionic Liquids and Metals Measured by Stark Shift Spectroscopy	Jahan Dawlaty USC
9:40	Extraordinarily Slow Dynamics in Thin Films of a Room Temperature Ionic Liquid Investigated with Reflection Geometry 2D IR Spectroscopy	Michael D. Fayer Stanford University
10:15	BREAK	
10:45	Selective Triplet-Initiated Intermolecular [2+2] Cycloadditions Photocatalyzed by Visible-light-Absorbing Quantum Dots	Emily A. Weiss Northwestern University
11:20	Characterization of Heterogenized CO ₂ Reduction Catalysis by Vibrational Sum-Frequency Spectroscopic, Electrochemical, and Theoretical Studies	Victor S. Batista Yale University
11:55	Photo/Electro-Catalytic Fuel Production from First Principles	Emily A. Carter Princeton University
12:30	LUNCH	
1:45	MURI on Molecular Level Studies of Solid-Liquid Interfaces in Electrochemical Processes	Tianquan Lian Emory University
2:20	Ultrafast Spectroscopy for Molecular Polariton and Atomic Specific Charge Dynamics	Wei Xiong UC San Diego
2:55	Generalized Einstein Relations Indicate Static Disorder in Perovskite Nanoplatelets	David M. Jonas University of Colorado
3:30	BREAK	
3:50	Artificial Atoms, Molecules, and Solids: Multiple Functions and Emergent Properties	Xiaoyang Zhu Columbia University
4:25	Many-Body Molecular Dynamics Simulations of Ionic Systems: From Clusters to Bulk and Interfaces	Francesco Paesani UC San Diego
5:00	Adjourn for dinner (not provided)	

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Agenda Day 2 | Wednesday, May 22, 2019

Time	Topic	Speaker
8:00	Registration	
8:30	Overview of Biological Sciences Research in the AFRL Materials and Manufacturing Directorate	Nancy Kelley-Loughnane AFRL
9:05	Conformational Motions and Electrostatics Facilitate Proton-Coupled Electron Transfer in BLUF Photoreceptor Proteins	Sharon Hammes-Schiffer Yale University
9:40	Cryptochrome-Based Magnetic Sensing	Peter J. Hore University of Oxford
10:15	BREAK	
10:45	Studies of metal oxide clusters and transient species with slow electron velocity-map imaging of cryogenically-cooled anions (cryo-SEVI)	Daniel Neumark UC Berkeley
11:20	Energetic and mechanistic information from temperature-dependent kinetics	Nicholas Shuman AFRL
11:55	Chemi-ionization Reactions of the Lanthanides and Their Potential as Catalysts: Guided Ion Beam and Theoretical Studies	Peter B. Armentrout University of Utah
12:30	LUNCH	
1:45	Density Matrix Renormalization Group Pair-Density Functional Theory for Excited States and Transition-Metal Compounds	Laura Gagliardi University of Minnesota
2:20	A View from Inside NSF Looking at AFOSR	F. Fleming Crim NSF
2:50	BREAK	
3:10	Program Status Update	Michael R. Berman AFOSR
3:30	POSTER SESSION	
5:00	Adjourn for dinner (not provided)	

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Agenda Day 3 | Thursday, May 23, 2019

Time	Topic	Speaker
8:00	Registration	
8:30	Nonequilibrium Dissociation in Hypersonic Flows using Computational Chemistry	Tom Schwartzentruber University of Minnesota
9:05	Studies of Dynamic Material Interfaces in Extreme Environments	Steven J. Sibener University of Chicago
9:40	Chemical Dynamics Simulations of Energy Transfer and Chemical Reaction in Collisions of $^3\text{O}_2$ with Graphite and of Gas-Phase Intermolecular Energy	William L. Hase Texas Tech University
10:15	BREAK	
10:45	Antenna-Reactors for Plasmonic Photocatalysis	Naomi J. Halas Rice University
11:20	Molecular-orbital-based machine learning for electronic structure	Thomas F. Miller III Caltech
11:55	Overview of Biological Sciences Research in the AFRL Human Performance Directorate	Rajesh Naik AFRL
12:30	LUNCH	
1:30	Electronic Structure and Nonadiabatic Dynamics for Reactions Near Surfaces and Gas-Metal Scattering	Joseph Subotnik U of Pennsylvania
2:05	Toward Ab Initio Molecular Dynamics on Many Electronic States	Benjamin G. Levine Michigan St. University
2:40	BREAK	
3:00	Modular Path Integral Methodology for Quantum Dynamics of Extended Systems	Nancy Makri University of Illinois
3:35	Plume Chemistry in the Space Environment	Christopher Annesley AFRL
4:10	MEETING ADJOURN	