

2021 AFOSR Molecular Dynamics and Theoretical Chemistry Program Review

Dr. Michael Berman | May 25-27, 2021 | Virtually

Agenda Day 1 | Tuesday, May 25, 2021 (Times are EDT)

Time	Topic	Speaker
9:30	Zoom Logon	
10:00	Intro Remarks	Michael R. Berman, AFOSR
10:10	Excitons and Trions in Colloidal Nanoplatelets as Qubits and Quantum Transduction Intermediates	Emily A. Weiss, Northwestern Univ
10:35	Tuning Mixing of Electronic and Vibrational States to Steer Excitonic Dynamics	Greg S. Engel, Univ of Chicago
11:00	BREAK	
11:20	Dynamics in Solids by Transient XUV Spectroscopy	Steven R. Leone, UC Berkeley
11:45	Theory and Simulation of Excitonic Complexes in Low-dimensional Materials	Timothy C. Berkelbach, Columbia Univ
12:10	Controlling Electron Dynamics at Semiconductor Surfaces by Molecular Functionalization Probed by XUV Reflection-Absorption Spectroscopy	L. Robert Baker, Ohio State Univ
12:35	BREAK	
1:45	A Possible Connection Between Relative Humidity, Aerosols, and Respiratory Infections	Richard N. Zare, Stanford Univ
2:10	Interfacial Electric Fields	Yogesh Surendranath, MIT
2:35	Heterogeneous Electrochemical Proton-Coupled Electron Transfer	Sharon Hammes-Schiffer, Yale Univ
3:00	BREAK	
3:20	Molecular Activation induced by Single Atomic Metal Anions and Metal Hydride Anions and a Progress Report on Cluster Models of Single Atom Catalysts	Kit Bowen, Johns Hopkins Univ
3:45	Atomically Dispersed Precious Metal Atoms as Active Sites on Plasmonic Photocatalysts	Phillip Christopher, UC Santa Barbara
4:15	MEETING ADJOURN	

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Agenda Day 2 | Wednesday, May 26, 2021 (Times are EDT)

Time	Topic	Speaker
9:30	Zoom Logon	
10:00	Intro Remarks	Michael R. Berman, AFOSR
10:10	Metal Chemistry in the Ionosphere	Nicholas Shuman, AFRL
10:35	Spectroscopy of Metal Oxide Space Clouds	Michael C. Heaven, Emory Univ
11:00	Lanthanide Cation Chemistry: Chemi-ionization Reactions, Spin Conservation, and Periodic Trends	Peter B. Armentrout, Univ of Utah
11:25	BREAK	
11:45	Fundamental Insights into Catalysis via Spectroscopy of Reactive Intermediates and Transition States	Daniel M. Neumark, UC Berkeley
12:10	Endothermic Reforming Using Novel Catalysts Prepared by Exsolution	Raymond J. Gorte, Univ of Pennsylvania
12:35	Small is Different: Cluster-Mediated Reactions	Uzi Landman, Georgia Tech
1:00	LUNCH	
2:00	Ice Nucleation Without Supercooling: On the Search for the Most Potent Ice Nucleants	Valeria Molinero, Univ of Utah
2:25	Nuclear Spin Conservation Enables State-to-State Control of Ultracold Molecular Reactions	Kang-Kuen Ni, Harvard Univ
2:50	BREAK	
3:15	Program Status Update	Michael R. Berman, AFOSR
3:40	Poster Session Demo	
4:00	Virtual Poster Session	
6:00	MEETING ADJOURN	

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Agenda Day 3 | Thursday, May 27, 2021 (Times are EDT)

Time	Topic	Speaker
9:30	Zoom Logon	
10:00	Intro Remarks	Michael R. Berman, AFOSR
10:10	Controlling Hot Electron Photoemission Dynamics in Plasmonic Nanostructures	David J. Nesbitt, Univ of Colorado
10:35	Mechanistic Insights into Plasmon Facilitated Catalysis: H ₂ Dissociation on Au Clusters	Hua Guo, Univ of New Mexico
11:00	Coupling between Molecular Excited States and Plasmons in Highly Confined Fields	Lasse Jensen, Penn State Univ
11:25	BREAK	
11:45	Progress Toward Imaging Chemical Dynamics in Ionic Liquid Electrolytes Using 2D IR Microscopy	Amber T. Krummel, Colorado State Univ
12:10	Ionic Liquids and their Applications in Propulsion	Adam Brand, AFRL
12:35	Dynamics of Ion Locking in Doubly Polymerized Ionic Liquids	Jennifer Laaser, Univ of Pittsburgh
1:00	LUNCH	
2:00	Molecular Beam Studies of Carbon Oxidation and Nitridation at High Temperatures	Timothy K. Minton, Univ of Colorado
2:25	Potential Energy Functions for High-energy Collisions of Atmospheric Gases and their Dissociation Products	Donald G. Truhlar, Univ of Minnesota
2:50	Progress in Gas-phase and Gas-surface Reaction Modeling for Hypersonic Flows	Thomas E. Schwartzentruber, Univ of Minnesota
3:15	BREAK	
3:30	Virtual Poster Session	
5:30	MEETING ADJOURN	