

2025 Molecular Dynamics and Theoretical Chemistry Program Review

Dr. Michael Berman | May 20-22, 2025 | Chantilly, VA -hybrid

Commercial Space Marketplace for Innovation and Collaboration (COSMIC)
14850 Conference Center Dr. | Suite 280 | Chantilly, VA 20151

Agenda Day 1 | May 20, 2025

Time	Topic	Speaker
8:00	Check-in / Login	
8:30	Toward Predictive Chemistry for Ionospheric Impacts of Novel Metals	Nicholas Shuman, AFRL
9:05	Understanding the Reactive Site in Catalysis through Spectroscopy of Clusters, Reactive Intermediates, and Transition States	Daniel Neumark, UC Berkeley
9:40	Ultrafast Reaction Dynamics Initiated by Chemically Relevant (70 eV) Electrons	Marcos Dantus, Michigan State University
10:15	BREAK	
10:45	Reactivity and Energy Dissipation for Energetic Gas-Surface Interactions	Steven Sibener, University of Chicago
11:20	Toward Photochemistry on Metal Nanoparticle Surfaces with Atomically Precise Active Sites	Phillip Christopher, University of California Santa Barbara
11:55	Sub-Nano Cluster Catalysts for Endothermic Cooling: Design Through Ensemble Representation	Anastassia Alexandrova, University of California, Los Angeles
12:30	LUNCH	
1:45	Water at the Edge: On-water Spectroscopy, Electrostatics and Chemistry	Wei Min, Columbia University
2:20	Chiral Phonon Contributions to Chiral Induced Spin Selectivity	Renee Frontiera, University of Minnesota
2:55	BREAK	
3:25	Chirality-Driven Magnetization Emerges from Relativistic Four-Current Dynamics	Xiaosong Li, University of Washington
4:00	Ultrafast XUV Spectroscopy Guides Chromophore and Photocatalyst Design	Josh Vura-Weis, University of Illinois at Urbana-Champaign
4:35	Discussion	
4:45	ADJOURN FOR DINNER (not provided)	

Agenda Day 2 | Wednesday, May 21, 2025

Time	Topic	Speaker
8:00	Check-in / Login	
8:30	Reaction Acceleration at the Air/Solution Interface of Microdroplets	Graham Cooks, Purdue University
9:05	Partial Solvation, Ionic Structure, and Chemical Reactions at the Air-Water Interface	Jahan Dawlaty, University of Southern California
9:40	Size-Dependent Condensation and Oxidation Reactions in Aqueous Microdroplets and Ice Grain Impact Phenomena	Robert Continetti, University of California San Diego
10:15	BREAK	
10:45	Deployable NMR Sensors Based on Spins out-of-Equilibrium	Ashok Ajoy, University of California Berkeley
11:20	Water Structuring on Polyvinyl Alcohol Surfaces Underlies Ice Recrystallization Inhibition	Songji Han, Northwestern University
11:55	Modular Real-time Path Integral Methods for Quantum Dynamics	Nancy Makri, University of Illinois at Urbana-Champaign
12:30	LUNCH	
1:45	Program Status Update	Michael Berman, AFOSR
2:20	Poster Session (See last pages of the agenda)	
4:45	ADJOURN FOR DINNER (not provided)	

Agenda Day 3 | May 22, 2025

Time	Topic	Speaker
8:00	Check-in / Login	
8:30	Structure and function of engineered surfaces of MXenes and MXenoids	Dmitri Talapin, University of Chicago
9:05	Combining Ab Initio Molecular Simulation and Machine Learning for Energetic Material Property Prediction	Edward Maginn, University of Notre Dame
9:40	Hypergolic Research at AFRL enabling "Green", Chemical Space Propulsion	Stefan Schneider, AFRL/RQRP (remote)
10:15	BREAK	
10:45	Mapping Potential-Dependent Molecular Dances Across an Electrochemical Cell	Amber Krummel, Colorado State University
11:20	Using Electrical Polarization in Understand and Control Thermochemical Surface Catalysis	Yogesh Surendranath, Massachusetts Institute of Technology
11:55	Molecular Activation and Single Atom Catalysis: Surface and Gas-Phase Studies	Kit Bowen, Johns Hopkins University
12:30	LUNCH	
1:30	Polaritonic Metastructures	Andrea Alu, City University of New York (remote)
2:05	Molecular Polariton Condensates	Vinod Menon, City College & Grad Center City University of New York
2:40	Real-Time Nuclear-Electronic Orbital Theory for Polaritons and Plasmons	Sharon Hammes-Schiffer, Princeton University
3:15	MEETING ADJOURN	

POSTER PRESENTATION ABSTRACTS

	Last Name	First Name	Title	Affiliation
1	Anderson	Scott	Developing and Validating Sub-Nano Catalysts for Endothermic Cooling: Experiments and DFT	University of Utah
2	Armentrout	Peter	Periodic Trends in Kinetic Energy Dependence, Reaction Efficiency, and Potential Energy Surface for Lanthanide Cation Oxidation in the Gas Phase by O ₂	University of Utah
3	Arnold	Michael	Photocurrent detection of polariton and exciton transfer: Uncovering energy and charge transport pathways and dynamics in photovoltaic materials	University of Wisconsin-Madison
4	Baker	Robert	A Materials Platform for Spin Selective Electrochemical Hydrogenation Catalysis	Ohio State University
5	Baker	Robert	Effect of Surface Electron Trapping and Small Polaron Formation on the Photocatalytic Efficiency of Copper(I) and Copper(II) Oxides	Ohio State University
6	Brorsen	Kurt	Connected-Triple Electronic Excitations in Quantum-Electrodynamics Coupled-Cluster Theory	University of Missouri
7	Crane	Matthew	Efficient hot carrier generation and transfer in low carrier concentration plasmonic nanomaterials	Colorado School of Mines
8	Dai	Hai Lung	The First Quantitative Measurement of Efflux Rates from Individual Compartments in Living Bacteria Cells – A study by Second Harmonic Light Scattering	Temple University
9	Dukovic	Gordana	Revealing the Phonon Bottleneck Limit in Negatively Charged CdS Quantum Dots	University of Colorado Boulder
10	Elliott	George	Training a Neural Network using EFMO	Iowa State University
11	Huo	Frank	Theory and Quantum Dynamics of Exciton Polariton transport	University of Rochester
12	Jackson	Megan	Measuring electric fields at gas-liquid interfaces	University of North Carolina at Chapel Hill
13	Jiang	Nan	Localized Surface Plasmon Controlled Chemistry at and beyond the Nanoscale	University of Illinois Chicago
14	Johnson	Mark	The onset for vibrationally-induced, intra-molecular proton transfer at three water molecules in microhydrated 4-aminobenzoic acid	Yale University
15	King	Sarah	Imaging of Surface Plasmon Polaritons in 2D Materials: From MXenes to Hyperbolic Materials	The University of Chicago
16	Knappenberger	Kenneth	Superatom magnetism and spin properties of colloidal metal clusters	Penn State University
17	Laskin	Julia	Understanding and controlling chemistry at interfaces using ion soft landing	Purdue university

18	Lee	Joonho	Structure and Dynamics of Charge Carriers Coupled to Lattice Vibrations	Harvard University
19	Leone	Stephen	Linear and Circular Dichroism of Core Excitons in LiF	University of California, Berkeley
20	Lewis	William	Online Chemical Analysis of Flowing Hydrocarbon Fuel Surrogates in a Pyrolysis Reactor by Optical Spectroscopy and Molecular Beam Mass Spectrometry	U.S. Air Force Research Laboratory
21	McDaniel	Jesse	Electrical Double Layer Modulation of Cation Radical Reaction Kinetics	Georgia Tech
22	Nuckolls	Colin	Coherent Transport of Energy and Information in 2D Superatomic Crystals	Columbia University
23	Roy	Xavier	Programmable transport in superatomic materials	Columbia University
24	Son	Minjung	Engineering photosynthetic energy transfer using polariton light-matter interactions	Boston University
25	Suits	Arthur	Crossed Beam Imaging of Associative Ionization and State-to-State Scattering Dynamics at High Collision Energy: Fundamental Studies for Hypersonics	Univ Missouri Columbia
26	Tang	MingLee	Chiroptical cavities for asymmetric synthesis with circularly polarized light	University of Utah
27	Thomas	Rich	Probing molecular mutual neutralization reactions of atmospheric importance using the ion storage facility DESIREE	Stockholm University
28	Vohs	John	Multicomponent Oxides for High-Temperature Catalysis	University of Pennsylvania
29	Weichman	Marissa	New Platforms for Molecular Polariton Dynamics	Princeton University
30	Zhang	Yingjie	Nucleation at solid-liquid interfaces is accompanied by the reconfiguration of electrical double layers	University of Illinois Urbana-Champaign