

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
4:45	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	
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	