

# 2024 AFOSR Molecular Dynamics and Theoretical Chemistry Program Review

Dr. Michael Berman | May 21-23, 2024 | Albuquerque, NM -hybrid

## Agenda Day 1 | 21 May 2024

Time	Topic	Speaker
8:00	Check in / Log on	
8:30	Attosecond XUV Probing of Spin Dynamics	Stephen Leone, UC Berkeley
9:05	TBD	Berkelbach, Columbia
9:40	Surface Plasmon Polaritons of MXenes	Sarah King, U Chicago
10:15	BREAK	
10:45	Hot Carrier Driven Processes on Electrode Surfaces	Tianquan (Tim) Lian, Emory
11:20	Chiroptical Excitation and Ultrafast Dynamics in Atomically Ordered Metals	Kenneth Knappenberger, Penn St
11:55	The Most Potent Snow Makers	Valeria Molinero, Utah
12:30	LUNCH	
1:45	Chiral Induced Spin Selectivity and Its Application for Spin Control in Redox Chemistry	David Waldeck, Pittsburgh
2:20	Towards a Fundamental Theory of the Chiral Induced Spin Selectivity Effect	Joseph Subotnik, U Penn
2:55	BREAK	
3:25	TBD	Nuckolls, Columbia
4:00	Inverse chirality-induced spin selectivity effect in chiral assemblies of $\pi$ -conjugated polymers	Dali Sun, NC State
5:00	Adjourn for dinner (not provided)	

Agenda Day 2   22 May 2024		
Time	Topic	Speaker
	<b>Registration</b>	
<b>8:30</b>	Molecular-level aspects of the electrostatic “reaction field” around solvated ionic structures through cryogenic spectroscopy	Mark Johnson, Yale
<b>9:05</b>	Role of Interfaces and Electrostatics for Chemical Transformations	Teresa Head-Gordon, UC Berk
<b>9:40</b>	Size-Dependent Condensation and Oxidation Reactions in Aqueous Microdroplets	Vicki Grassian, UCSD
<b>10:15</b>	<b>BREAK</b>	
<b>10:45</b>	Recent Progress of Polariton Chemistry Research	Wei Xiong, UCSD
<b>11:20</b>	Molecular Cavity Quantum Electrodynamics and Polariton Chemistry	Frank Huo, Rochester
<b>11:55</b>	Photocurrent readout of polaritons: Physical evidence for long range exciton transfer	Mike Arnold, University of Wisconsin-Madison
<b>12:30</b>	<b>LUNCH</b>	
<b>1:45</b>	TBD	Prince, AFRL
<b>2:20</b>	Program Status Update	Michael Berman, AFOSR
<b>2:55</b>	<b>BREAK</b>	
<b>3:10</b>	Poster Session	
<b>5:00</b>	<b>Adjourn for dinner (not provided)</b>	

Agenda Day 3   23 May 2024		
Time	Topic	Speaker
	<b>Registration</b>	
8:30	Dynamics, Structure, and Interactions in Thin Films and Bulk RTILs	Michael Fayer, Stanford
9:05	Plasmon-enhanced photocatalysis for green and sustainable hydrogen production	Peter Nordlander, Rice
9:40	Ultrafast Hot Electron Cooling Dynamics in Plasmonic Nanostructures and Single Molecule Biophysics of Riboswitch Folding	David Nesbitt, Colorado
10:15	<b>BREAK</b>	
10:45	A General Method for Single Molecule Spectroscopy	David Patterson, UCSB
11:20	Quantum Chemistry for Quantum Logic	Eric Hudson, UCLA
11:55	Quantum Wigner molecules in semi-conductor quantum dots, TMD moiré materials & their superlattices, and polymeric electron zig-zag chains in inter quantum-dot couplers	Uzi Landman, Georgia Tech
12:30	<b>LUNCH</b>	
1:30	Exploring Multimetallic Molecules with Localized Multireference Methods	Laura Gagliardi, Chicago
2:05	Non-Equilibrium Flow Experiments in the GALCIT T5 Reflected Shock Tunnel: Aerothermochemistry Measurements and Modeling	Christopher Strand, Stanford
2:40	<b>BREAK</b>	
3:10	TBD	Vojvodic, U Penn
3:45	Stabilizing sub-nano catalysts for high temperature reactions of interest for fuel cooling	Scott Anderson, Utah
4:20	<b>Meeting Ends</b>	