

2024 AFOSR Molecular Dynamics and Theoretical Chemistry Program Review

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

University of New Mexico Rotunda
The Rotunda is located at 801 University Blvd. SE, Albuquerque, NM 87106

Agenda Day 1 | May 21, 2024

| Time | Topic | Speaker |
|-------|--|-----------------------------------|
| 8:00 | Check in / Log on | |
| 8:25 | Opening Remarks | Michael Berman, AFOSR |
| 8:30 | Attosecond XUV Probing of Spin Dynamics | Stephen Leone, UC Berkeley |
| 9:05 | Ab initio surface chemistry with chemical accuracy | Timothy 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 State |
| 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 | Chiroptics and spin selectivity in helicenes and twistacenes | Colin Nuckolls, Columbia |
| 4:00 | Inverse chirality-induced spin selectivity effect in chiral assemblies of π -conjugated polymers | Dali Sun, NC State |
| 5:00 | Adjourn for dinner (not provided) | |

Agenda Day 2 | May 22, 2024

| Time | Topic | Speaker |
|-------|---|--|
| 8:00 | Check in / Log on | |
| 8:25 | Opening Remarks | Michael Berman, AFOSR |
| 8:30 | Molecular-level aspects of the electrostatic “reaction field” around solvated ionic structures through cryogenic spectroscopy | Mark Johnson, Yale |
| 9:05 | Role of Interfaces and Electrostatics for Chemical Transformations | Teresa Head-Gordon, UC Berkeley |
| 9:40 | Size-Dependent Condensation and Oxidation Reactions in Aqueous Microdroplets | Vicki Grassian, UCSD |
| 10:15 | BREAK | |
| 10:45 | Recent Progress of Polariton Chemistry Research | Wei Xiong, UCSD |
| 11:20 | Molecular Cavity Quantum Electrodynamics and Polariton Chemistry | Frank Huo, Rochester |
| 11:55 | Photocurrent readout of polaritons: Physical evidence for long range exciton transfer | Mike Arnold, University of Wisconsin-Madison |
| 12:30 | LUNCH | |
| 1:45 | Characterizing nanodroplets of ionic liquid electrospray thrusters – mass, charge, plume effects and contamination | Benjamin Prince, AFRL |
| 2:20 | Program Status Update | Michael Berman, AFOSR |
| 2:55 | BREAK | |
| 3:10 | Poster Session | |
| 5:00 | Adjourn for dinner (not provided) | |

Agenda Day 3 | May 23, 2024

| Time | Topic | Speaker |
|-------|---|------------------------------|
| 8:00 | Check in / Log on | |
| 8:25 | Opening Remarks | Michael Berman, AFOSR |
| 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 | BREAK | |
| 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 | LUNCH | |
| 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 | BREAK | |
| 3:10 | Tailoring Metal-Oxide Interactions for Enhanced Catalytic Activity and Stability | Aleksandra Vojvodic, U Penn |
| 3:45 | Stabilizing sub-nano catalysts for high temperature reactions of interest for fuel cooling | Scott Anderson, Utah |
| 4:20 | MEETING ENDS | |