

# MOLECULAR DYNAMICS AND THEORETICAL CHEMISTRY PROGRAM REVIEW

Dr. Michael Berman | May 24-26, 2016 | Arlington, VA

## Basic Research Innovation Collaboration Center BRICC

4075 Wilson Blvd, Suite 350, Liberty Room  
Arlington VA 22203

### AGENDA Day 1 – Tuesday, May 24, 2016

Time	Title of Project	Speaker
8:00-8:20	Registration/ Admin/Speaker Set-Up	
8:20-8:30	Welcome and Introductory Remarks	<b>Michael Berman,</b> Air Force Office of Scientific Research
8:30-9:05	Microdroplet Chemistry	<b>Richard Zare,</b> Stanford University
9:05-9:40	Nanochemical Strategies for Propulsion Enhancement	<b>Scott Anderson,</b> University of Utah
9:40-10:15	Chemical Dynamics Associated with Electric Space Propulsion	<b>Benjamin D. Prince,</b> AFRL
10:15-10:45	<b>BREAK</b>	
10:45-11:20	Structure and Reactivity of Transient Species in Water Splitting and CO <sub>2</sub> Reduction Using Cryogenic Ion Spectroscopy	<b>Mark Johnson,</b> Yale University
11:20-11:55	Tabletop M-edge XANES Spectroscopy of Molecular Transition Metal Complexes	<b>Josh Vura-Weis,</b> University of Illinois at Urbana-Champaign
11:55-12:30	Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer	<b>Sharon Hammes-Schiffer,</b> University of Illinois at Urbana-Champaign
12:30-2:00	<b>LUNCH</b>	
2:00-2:35	Plasmon-induced Hot Carrier Photocatalysis	<b>Naomi Halas,</b> Rice University
2:35-3:15	Elucidating the Specific Role of Metal SPR in Enhancing Surface Photochemistry	<b>Wei David Wei,</b> University of Florida
3:15-3:35	<b>BREAK</b>	
3:35-4:10	Velocity Map Photoelectron Imaging and Ultrafast Dynamics of Plasmonic Nanostructures	<b>David Nesbitt,</b> University of Colorado
4:10-4:45	Electron Dynamics in Super-Atom and Hybrid Semiconductors	<b>Xiaoyang Zhu,</b> Columbia University
4:45	<b>ADJOURN FOR THE DAY</b>	

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### AGENDA Day 2 – Wednesday, May 25, 2016

Time	Title of Project	Speaker
8:00-8:30	Registration/ Admin/Speaker Set-Up	
8:30-9:05	Improving the flow and measurement of energy transport in semiconducting carbon nanotube devices	<b>Martin Zanni</b> , University of Wisconsin
9:05-9:40	Impact of surface chemistry of semiconductor nanocrystals on their photophysics and photochemistry	<b>Gordana Dukovic</b> , University of Colorado
9:40-10:15	Mechanistic Insights into CO <sub>2</sub> Reduction on Semiconductor Photoelectrodes	<b>Emily Carter</b> , Princeton University
10:15-10:45	<b>BREAK</b>	
10:45-11:20	A Surface Hopping Picture of Electrochemistry	<b>Joseph Subotnik</b> , University of Pennsylvania
11:20-11:55	Chemical releases, transition metal kinetics, and fundamental ion chemistry	<b>Nicholas Shuman</b> and <b>Albert Viggiano</b> , Air Force Research Laboratory
11:55-12:30	Advanced Electronic Structure Methods for Heavy-Element Chemistry	<b>Toru Shiozaki</b> , Northwestern University
12:30-2:00	<b>LUNCH</b>	
2:00-2:35	Nonequilibrium Dissociation Model from Direct Molecular Simulation	<b>Thomas Schwartzentruber</b> , University of Minnesota
2:35-3:15	Probing Pyrolysis in the Condensed Phase: One and Two Component Fluid Compositions	<b>Christopher Bunker</b> , Air Force Research Laboratory
3:15-3:35	<b>BREAK</b>	
3:35-4:15	Program Status Update, Molecular Dynamics and Theoretical Chemistry	<b>Michael Berman</b> , AFOSR
4:15	<b>POSTER SESSION</b>	
TBD	<b>ADJOURN FOR THE DAY</b>	

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### AGENDA Day 3 – Thursday, May 26, 2016

Time	Title of Project	Speaker
8:00-8:30	Registration/ Admin/Speaker Set-Up	
8:30-9:05	Can Vibronic Resonances Control Energy Transfer?	David M. Jonas University of Colorado
9:05-9:40	Ultrafast Photoinduced Interfacial Proton-Coupled Electron Transfer	Tianquan Lian, Emory University
9:40-10:15	Dynamics of Electron Emission into Water	Robert Hamers, University of Wisconsin
10:15-10:45	BREAK	
10:45-11:20	Toward the Development of Aluminum Cluster-Containing Materials for Propulsion Applications	Kit Bowen, Johns Hopkins University
11:20-11:55	Cluster Films by Helium Droplet Mediated Cluster Assembly: Growth and Characterization	Michael Lindsay AFRL
11:55-12:30	Theoretical studies of nanocluster formation	Jerry Boatz, AFRL
12:30	MEETING ADJOURNED	