



### Key Bridge Marriott Hotel

1401 Lee Highway  
Arlington, VA 22209

### AGENDA Day 1 – Tuesday, May 22, 2012

Time	Title of Project	Speaker
7:00-8:25	Registration	
8:25-8:30	Opening Remarks	<b>Michael Berman</b> , Air Force Office of Scientific Research
8:30-9:05	Cluster Dynamics: Laying the Foundation for Tailoring the Design of Cluster Assembled Nanoscale Materials	<b>Will Castleman</b> , Penn State University
9:05-9:40	Model Catalysts and Nanoparticles for Propulsion Applications	<b>Scott Anderson</b> , University of Utah
9:40-10:15	Neutral Cluster Heterogeneous Catalysis: New Systems, Supported Species, Mechanisms	<b>Elliott Bernstein</b> , Colorado State University
10:15-10:45	<b>BREAK</b>	
10:45-11:20	Ultrafast High Harmonic, Soft X-Ray Laser Probing of Molecular Dynamics	<b>Stephen Leone</b> , University of California - Berkeley
11:20-11:55	Size Matters: Photophysical Properties of Nanoclusters	<b>Ruth Pachter</b> , AFRL
11:55-12:30	Computationally Guided Materials Design via Coarse-Graining	<b>Greg Voth</b> , University of Chicago
12:30-1:55	<b>LUNCH</b>	
2:00-2:35	Using Vibrations to Probe and Control Photoisomerization in Liquids	<b>Fleming Crim</b> , University of Wisconsin - Madison
2:35-3:10	Nanoscale Dynamics and Spectroscopy in Extreme Environments	<b>Kenneth Knappenberger</b> , Florida State University
3:10-3:45	Nano-Scale Energetic Films by Superfluid Helium Droplet Assembly	<b>C. Michael Lindsay</b> , AFRL
3:45-4:15	<b>BREAK</b>	
4:15-5:00	Electrochemistry Discussion	
5:00-7:00	<b>ADJOURN FOR DINNER (NOT PROVIDED)</b>	
7:00-9:00	<b>POSTER SESSION</b>	



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### AGENDA Day 2 – [Wednesday, May 23, 2012](#)

Time	Title of Project	Speaker
7:30-8:30	Registration	
8:30-9:05	Investigating Catalytic Processes using Mass Spectrometry	<b>Richard Zare</b> , Stanford University
9:05-9:40	Photoinduced Proton-Coupled Electron Transfer Reactions: Electron-Proton Nonadiabaticity and Ultrafast Dynamics	<b>Sharon Hammes-Schiffer</b> , Pennsylvania State University
9:40-10:15	How Changing the Number of Electrons Opens the Door to Routine, Multi-Reference Coupled-Cluster Applications	<b>Rodney Bartlett</b> , University of Florida
10:15-10:45	<b>BREAK</b>	
10:45-11:20	Charge & Field Effects in Clusters: Nanocatalysis, Water Nanodrops, Electrocrystalliation and Proton-Coupled Electron Transfer in DNA	<b>Uzi Landman</b> , Georgia Institute of Technology
11:20-11:55	Novel Catalytic Mechanisms for the Chemical Reduction of Carbon Dioxide to Energy-Dense Liquids (MURI)	<b>Emily Carter</b> , Princeton University
11:55-12:30	Ultrafast and Diffusion-Limited Charge Extraction from PbS Quantum Dots Gated by the Native Ligand Shell	<b>Emily Weiss</b> , Northwestern University
12:30-2:00	<b>LUNCH</b>	
2:00-2:35	Thermodynamics of Isolated Bi-Atomic Clusters	<b>Garth Wilks</b> , AFRL
2:35-3:10	Efficient Methods for Exploring Potential Energy Surfaces of Chemical Reactions and Discovery of Excited Roaming Pathways for NO <sub>3</sub> Photodissociation and Chirality Control in the Growth on Carbon Nanotubes	<b>Keiji Morokuma</b> , Emory University
3:10-3:45	Structure-Property Relationships in Nanostructured Electrodes for Hybrid Photovoltaics and Batteries	<b>Michael Durstock</b> , AFRL
3:45-4:15	<b>BREAK</b>	
4:15-5:00	Program Status Update	<b>Michael Berman</b> , Air Force Office of Scientific Research
5:00	<b>ADJOURN FOR THE DAY</b>	



# Molecular Dynamics Program Review

Dr. Michael Berman | 22-24 May 2012 | Arlington, VA

## Key Bridge Marriott Hotel

1401 Lee Highway  
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### AGENDA Day 3 – Thursday, May 24, 2012

Time	Title of Project	Speaker
7:30-8:30	Registration	
8:30-9:05	Extremes in Oxidizing Power, Acidity and Basicity	Josef Michl, University of Colorado
9:05-9:40	Novel Catalytic Synthetic Methods for Main Group Materials and Reagents for Organic Synthesis	John Arnold, University of California - Berkeley
9:40-10:15	Polynitrogen and High-Nitrogen Chemistry	Karl Christe, University of Southern California
10:15-10:45	BREAK	
10:45-11:20	Theoretical Studies of Gas-Surface and Gas-Phase Dynamical Processes	George Schatz, Northwestern University
11:20-11:55	Spectroscopy of Gas-Phase Ionic Liquids	Jamie Stearns, AFRL
11:55-12:30	Size and Composition Optimized Nanocatalysts for Propulsion Applications	Lisa Pfefferle, Yale University
12:30-2:00	CLOSING REMARKS/ADJORN/LUNCH	
2:00-4:00	OPTIONAL OPEN DISCUSSIONS	
		New Research Directions Hot Topics New Processes
4:00	OPTIONAL DISCUSSIONS ADJOURNED	