



### 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	<a href="#">Cluster Dynamics: Laying the Foundation for Tailoring the Design of Cluster Assembled Nanoscale Materials</a>	<b>Will Castleman</b> , Penn State University
9:05-9:40	<a href="#">Model Catalysts and Nanoparticles for Propulsion Applications</a>	<b>Scott Anderson</b> , University of Utah
9:40-10:15	<a href="#">Neutral Cluster Heterogeneous Catalysis: New Systems, Supported Species, Mechanisms</a>	<b>Elliott Bernstein</b> , Colorado State University
10:15-10:45	<b>BREAK</b>	
10:45-11:20	<a href="#">Ultrafast High Harmonic, Soft X-Ray Laser Probing of Molecular Dynamics</a>	<b>Stephen Leone</b> , University of California - Berkeley
11:20-11:55	<a href="#">Size Matters: Photophysical Properties of Nanoclusters</a>	<b>Ruth Pachter</b> , AFRL
11:55-12:30	<a href="#">Computationally Guided Materials Design via Coarse-Graining</a>	<b>Greg Voth</b> , University of Chicago
12:30-1:55	<b>LUNCH</b>	
2:00-2:35	<a href="#">Using Vibrations to Probe and Control Photoisomerization in Liquids</a>	<b>Fleming Crim</b> , University of Wisconsin - Madison
2:35-3:10	<a href="#">Nanoscale Dynamics and Spectroscopy in Extreme Environments</a>	<b>Kenneth Knappenberger</b> , Florida State University
3:10-3:45	<a href="#">Nano-Scale Energetic Films by Superfluid Helium Droplet Assembly</a>	<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	<a href="#">Investigating Catalytic Processes using Mass Spectrometry</a>	<b>Richard Zare,</b> Stanford University
9:05-9:40	<a href="#">Photoinduced Proton-Coupled Electron Transfer Reactions: Electron-Proton Nonadiabaticity and Ultrafast Dynamics</a>	<b>Sharon Hammes-Schiffer,</b> Pennsylvania State University
9:40-10:15	<a href="#">How Changing the Number of Electrons Opens the Door to Routine, Multi-Reference Coupled-Cluster Applications</a>	<b>Rodney Bartlett,</b> University of Florida
10:15-10:45	<b>BREAK</b>	
10:45-11:20	<a href="#">Charge &amp; Field Effects in Clusters: Nanocatalysis, Water Nanodrops, Electrocrystalliation and Proton-Coupled Electron Transfer in DNA</a>	<b>Uzi Landman,</b> Georgia Institute of Technology
11:20-11:55	<a href="#">Novel Catalytic Mechanisms for the Chemical Reduction of Carbon Dioxide to Energy-Dense Liquids (MURI)</a>	<b>Emily Carter,</b> Princeton University
11:55-12:30	<a href="#">Ultrafast and Diffusion-Limited Charge Extraction from PbS Quantum Dots Gated by the Native Ligand Shell</a>	<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	<a href="#">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</a>	<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>	



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