

ARO Workshop on Roaming and Cold Molecules  
Emory University, 360 Atwood Hall

Schedule for **SATURDAY**, Oct. 8, 2016

AM Session Chairs: Craig Murray and Phillip Stancil

8:30 – 9:00	Continental Breakfast, Lobby outside of seminar room	
9:05 – 9:35	Roaming Under the Microscope: Trajectory Study of Formaldehyde Dissociation	Paul Houston
9:35 – 10:05	Roaming Mechanisms for Nitrogen Containing Compounds: $\text{CH}_3\text{NO}_2$ , $(\text{CH}_3)_2\text{NNH}_2$ , $\text{CH}_3\text{NH}(\text{NO}_2)$ , and $\text{HNNOH}$	Stephen Klippenstein
10:10 – 10:35	Break (Refreshments), Lobby	
10:45 – 11:15	Patterns, Broken Patterns, and Broken Patterns of Broken Patterns	Bob Field
11:15 – 11:45	Rotationally Resolving Large Buffer-Gas Cooled Molecules In The Mid-infrared With Direct Frequency Comb Spectroscopy	Ben Spaun
11:45-noon	Additional discussion	
Noon – 1:30	Lunch in Emory Village	

PM Session Chairs: Joel Bowman and Balakrishnan Naduvalath

1:30 – 2:00	Towards Quantum-State-Resolved Charged-Neutral Chemistry	Eric Hudson
2:00 – 2:30	Competing Pathways in the Near-UV Photodissociation of Acetaldehyde	Craig Murray
2:30 – 3:00	Geometric Phase Effects Associated with Conical Intersections in the Ultracold Regime	Svetlana Kotochigova
3:00 – 3:30	Break (Refreshments)	
3:30 – 4:00	Roaming Signature in Photodissociation of Some Carbonyl Compounds	King-Chuen Lin
4:00 – 4:30	Quantum Dynamics of Cold Inelastic Diatom-Diatom Collisions in Full Dimensionality	Phillip Stancil
4:30 – 5:00	Roaming: Dynamical Reaction Pathways in Phase Space	Stephen Wiggins
6:30	Cocktails (cash bar) for all in the Starvine Ballroom at the Emory Conference Center Hotel (ECCH)	
7:00	Dinner for all registered, in the ECCH Starvine Ballroom	

ARO Workshop on Roaming and Cold Molecules Emory University, 360 Atwood Hall  Schedule for <b>SUNDAY</b> , Oct. 9, 2016		
AM Session Chairs: Gary Douberly and Francesco Evangelista		
8:00 – 8:30	Continental Breakfast	
8:30 – 9:00	Direct Dynamics Simulations of the Role of Microsolvation in $S_N2$ Reactions. Consideration of the Theoretical Method, Zero Point Energy, and Experiment	Bill Hase
9:00 – 9:30	Two-electron Reduced Density Matrices in Electronic Structure and Dynamics	David Mazziotti
9:30 – 10:00	Molecular Alignment Effect on the Photoassociation Process via a Pump-Dump Scheme	Yonchang Han
10:00 – 10:30	Break (Refreshments)	
10:30 – 11:00	Control of Roaming in Complex Organic Reactions in Solution	Dan Singleton
11:00 – 11:30	Including Roaming Trajectories Within the TST fold.	Rigoberto Hernandez
11:30-noon	Additional discussion	
Noon – 1:30	Lunch in Emory Village	
PM Session Chair: Michael Heaven		
1:30 – 2:00	Roaming in Coulomb Crystals	Ken Brown
2:00 – 2:30	Roaming in Biomolecular Reactions	Arthur Suits
2:30 – 3:00	Wrap up	

Onsite contact: Susan Browne, 404-377-6117 (cell), [sebrown@emory.edu](mailto:sebrown@emory.edu)