

Spectroscopy and Dynamics on Multiple Potential Energy Surfaces
Organizers: Michael Heaven, Anne McCoy, Scott Reid, Trevor Sears
Location: Telluride Intermediate School, 725 W. Colorado Ave, Telluride CO 81435
TSRC Hosts: Mark Kozak, Executive Director, 970.708.4226
Cindy Fusting, Managing Director, 970.708.5069 or Kristen Redd, Lodging Director, 970.729.8375

Monday, July 16th

- Arrive, informal gathering at Smugglers at 6 pm - ??

Tuesday, July 17th

- MORNING SESSION: Trevor Sears, Chair
 - 7:45 Breakfast at TSRC
 - 8:15 Announcements
 - 8:20 **Anne McCoy** (University of Washington)
Sorting out vibrational couplings in protonated water cluster ions
 - 8:55 **Ken McKendrick** (Heriot-Watt University)
Probing liquid surfaces using reactive-atom scattering
 - 9:30 BREAK
 - 9:50 **Dan Neumark** (UC-Berkeley)
Studies of free radicals, clusters, and transition states using slow electron velocity-map imaging of cryogenically cooled anions
 - 10:25 **Marsha Lester** (University of Pennsylvania)
Spectroscopy and unimolecular decay dynamics of Criegee intermediates
 - 11:00 BREAK
 - 11:20 **Timothy Schmidt** (University of New South Wales)
Singlet fission: It's a Trap! And musings on electronic structure
 - 11:55 **Richard Dawes** (Missouri Institute of Science and Technology)
AUTOSURF: automated construction of PESs with direct interface to variational rovibrational calculations
 - 12:30 Session concludes
- AFTERNOON FREE
- EVENING
 - 6:00 Town Talk, Telluride Conference Center, Mountain Village
Pavel Jungwirth, *The Explosiveness of Salt*

Wednesday, July 18th

- MORNING FREE
 - AFTERNOON SESSION: Scott Reid, Chair
 - 1:15 Announcements
 - 1:20 **Scott Kable** (University of New South Wales)
The oft-forgotten role of the ground state in carbonyl photolysis
 - 1:55 **Lyudmila Slipchenko** (Purdue University)
Excitonic triplet-triplet coupling in chromophore dimers
 - 2:30 **Curt Wittig** (University of Southern California)
He in liquid helium: spherical cows, adiabaticity, exciton transport, and a mysterious ion*
 - 3:05 BREAK
 - 3:25 **Terry Miller** (The Ohio State University)
The Jahn-Teller Effect and Degeneracy Breaking in Isolated Molecules: Experimental Observables and Results
 - 4:00 **John Stanton** (University of Florida)
The ²E'' Excited State of NO₃: A Discussion of Theoretical Challenges and Some Results
 - 4:35 session ends
 - EVENING
 - 6:00 Picnic, Under the tent at TSRC, 725 W Colorado Avenue
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Thursday, July 19th

- MORNING FREE
 - AFTERNOON SESSION: Anne McCoy, Chair
 - 1:15 Announcements
 - 1:20 **Michael Heaven** (Emory University)
Beryllium bonding probed by anion photodetachment
 - 1:55 **David Osborn** (Sandia National Laboratories)
Photodissociation of Acetyl Acetone: much more than just OH
 - 2:30 **Tim Zwier** (Purdue University)
The Spectroscopy of Open-shell radicals and Flexible Bichromophores
 - 3:05 BREAK
 - 3:25 **Lan Cheng** (Johns Hopkins University)
Accurate ab initio calculations for low-lying electronic states in heavy-metal containing molecules: spin-orbit coupling and magnetic properties
 - 4:00 **Tim Steimle** (Arizona State University)
Polyatomic heavy element radical molecules as a venue for fundamental physics
 - 4:35 Session concludes
 - EVENING SESSION: Michael Heaven, Chair
 - 7:00 **Millard Alexander** (University of Maryland)
Spin-orbit Branching in Molecular Photodissociation
 - 7:35 **Trevor Sears** (Brookhaven/Stony Brook)
New Insights into the Spectroscopy and Dynamics of the CCH Radical
 - 8:10 **Craig Taatjes** (Sandia National Laboratory)
Hydrocarbon oxidation and reactions on multiple potential energy surfaces
 - 8:45 Session Concludes
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Friday, July 20th

- MORNING: TBD, Chair
 - 10:30 Announcements
 - 10:35 **Craig Murray** (UC-Irvine)
Photodissociation dynamics of organic carbonyls and their cations
 - 11:10 **Greg Hall** (Brookhaven National Laboratory)
Collisional effects in lineshapes and line shifts: Stringent tests of potential energy surfaces
 - 11:45 **Ned Sibert** (University of Wisconsin)
Theoretical attempts to model the benzene-water and propylbenzene-water OH stretch spectra.
 - 12:20 Session Concludes
 - AFTERNOON: TBD, Chair
 - 2:00 Announcements
 - 2:05 **Spiridoula Matsika** (Temple University)
Nonadiabatic effects in photon and electron driven reactions
 - 2:40 **Paul Dagdigan** (Johns Hopkins University)
Inelastic and Reactive Collisions of Astrophysical Molecules
 - 3:15 **Jingsong Zhang** (UC-Riverside)
Excited-state dynamics and photodissociation of small free radicals
 - 3:50 BREAK
 - 4:10 **Meredith Jordan** (University of Sydney)
Inter-System Crossing in Carbonyls
 - 4:35 **Scott Reid** (Marquette University)
Exciton coupling in fluorene-based bichromophores: Vibrational quenching
 - 5:10 Session Concludes
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