***New Challenges for Theory in Chemical Dynamics***

*Telluride Winter Workshop, Jan 12–17, 2014*

*Ah Haa School for the Arts, 300 S. Townsend, Telluride*

*Millard Alexander, Chair (301-785–4791)*

*Nana Naisbitt, Director, TSRC (970-708-0004)*

**Sunday, Jan 12:**

*6:00–8:00 PM, Registration and informal gathering, Arroyo Wine Bar, 220 E Colorado Avenue, Cash Bar, Wine Specials, Appetizers complements of Millard*

**Monday, Jan 13:**

*7:15–8:15am Breakfast, Ah Haa School for the Arts,*

*Registration/Check-in for later comers*

Session MM (Morning), Ah Haa School for the Arts

Chair:  M. Alexander

8:15am Opening remarks

8:30–9:15am John Stanton, University of Texas

NO3 and Vibronic Coupling

9:15–10:00am Bill Poirier, Texas Tech University

Ten Thousand Quantum States of Acetonitrile

10:00–10:30am coffee break

10:30–11:15am Tucker Carrington, Queens University

Calculating the ro-vibrational spectrum of methane and refining its potential energy surface

*Dinner, 5:30 PM. Floradora Saloon, 103 W. Colorado Ave., 970 728-8884, Individual tabs*

Session ME   (Evening), Ah Haa School for the Arts

Chair:  H. Guo

7:15–8:00pm Dmitri Babikov, Marquette University

Mixed Quantum/Classical Theory of Collisional Energy Transfer

8:00–8:45pm Haobin Wang, New Mexico State University

Effect of correlation in quantum transport

**Tuesday, Jan 14:**

*7:15–8:15am Breakfast, Ah Haa School for the Arts*

Session TM  (Morning)

Chair: P. Dagdigian

8:30–9:15am François Lique, University le Havre (FR)

Collisional excitation of CN and O2 by H2 : Fine-structure resolved transitions and comparison with experiments

9:15–10:00am Hua Guo, University of New Mexico

Predicting mode/bond selectivity and energy disposal in bimolecular reactions from the sudden perspective

10:00–10:30am coffee break

10:30–11:15am Andreas Osterwalder, EPFL, Lausanne (CH)

Experimental studies of low-temperature reactive scattering

*5:10pm pick up from AhHaa School for dinner, TSRC Sponsored Party at Mountain Village home of Audrey Marnoy, Board of Directors*

Session TE  (Evening), AhHaa School for the Arts

Chair:  F. Lique

8:00–8:45pm Donghui Zhang, Dalian Institute for Chemical Physics (CN),

Theoretical Studies of Polyatomic Reaction Dynamics

8:45–9:30pm Richard Dawes, University of Missouri

Electronic structure considerations for global potential energy surfaces

**Wednesday, Jan 15:**

*7:15–8:15am Breakfast, AhHaa School for the Arts,*

Session WM (Morning)

Chair:  W. Thompson

8:30–9:15am Vladimir Mandelshtam, University of California, Irvine

Anomalous quantum and isotope effects in water clusters: A physical phenomenon or model artifact?

9:15–10:00am Toshiyuki Takayanagi, Saitama University (JP)

Dynamics study of excess electron attachment to molecules and clusters

10:00-10:30am coffee break

10:30–11:15am Rigoberto Hernandez, Georgia Tech University

Adaptive steering molecular dynamics (ASMD): Unfolding of Neuropeptide Y and deca-alanine stretching

11:15am–12:00pm David Coker, Boston University

Iterative linearized and partial linearized density matrix dynamics: Applications to energy and electron transfer

*5:30 – 7:45 Conference dinner, Chop House Restaurant, New Sheridan Hotel, 231 West*

*Colorado Avenue (970) 728-4351*

Session WE  (Evening)

Chair:  B. Poirier

8:00–8:45pm Millard Alexander, University of Maryland

Rotational, Electronic, and Vibrational Energy flow in Methylene

8:45–9:30pm Amy Mullin, University of Maryland

Collision dynamics of molecular gyroscopes

**Thursday, Jan 10:**

*7:15–8:15am Breakfast, Ah Haa School for the Arts,*

Session ThM (Morning)

Chair:  R. Dawes

8:30–9:15am Jacek Klos, University of Maryland

Tests of ab initio potentials in chemical dynamics of the OH–H2 and He\*–H2/HD/D2 systems

9:15–10:00am  Zlatko Bacic, New York University

Hydrogen molecules in nanoscale cavities: Quantum dynamics, inelastic neutron scattering spectroscopy, and an unexpected selection rule for H2/HD in C60

10:00–10:30am coffee break

10:30–11:15am Ward Thompson, University of Kansas

Dynamics of Nanoconfined Liquids

Session ThA (Afternoon)

Chair:  T. Carrington

4:00–4:45pm Paul Dagdigian, The Johns Hopkins University,

Quantum Scattering Calculations of Transport Properties

4:45–5:30pm Pierre-Nicolas Roy, University of Waterloo (CA)

Path integral simulations of complex molecular systems

*6:00 – 8:00pm Dinner Rustico Restorante, 114 East Colorado Ave*

Session ThE (Evening) New Sheridan Bar

Off-the-wall idea session and get together

**Friday, Jan 11:**

*7:30am (Morning) Informal Breakfast, Baked in Telluride, 127 S Fir St*