**Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems**

**Telluride Workshop, July 13–18, 2014**

**Organizers: Zlatko Bačić, Tucker Carrington, Mark Tuckerman**

**TSRC hosts: Nana Naisbitt (970-708-0004) and Rory Sullivan (970-708-4542)**

**Meeting location: Telluride Intermediate School at 725 W. Colorado Ave.**

**Sunday, July 13:**

8:00:10:00 pm: Registration and informal gathering, Arroyo Wine Bar, 220 E Colorado Avenue. Cash bar, wine specials, appetizers will be served compliments of your organizers.

**Monday, July 14:**

7:30–8:15 am: Breakfast at TSRC, Registration/Check-in for late-comers

8:15–8:30 am: Opening remarks

Session I (Morning), TSRC

**Chair:** Dominik Marx, Ruhr-Universität, Bochum

8:30–9:15 am: Joel Bowman, Emory University

*“The effect of large-amplitude motion on O-H and H-Cl stretches in clusters: quantum calculations using ab initio potential energy surfaces.”*

9:15–10:00 am: Martin Suhm, Georg-August Universität

*“OH stretching anharmonicities and couplings in hydrogen-bonded clusters: Fairly stiff yardsticks from vibrational jet spectroscopy.”*

10:00–10:30 am: Coffee Break

     10:30–11:15 am: Claude Leforestier, Université Montpellier

“*Infrared shifts calculation of water clusters****.”***

11:15 am –12:00 pm: Francesco Paesani, University of California San Diego

“*Vibrational spectroscopy of water in metal-organic frameworks****.”***

12:00–2:00 pm: Lunch, on your own.

Session II (Afternoon), TSRC

**Chair:** Motoyuki Shiga, Japan Atomic Energy Agency

2:00–2:45 pm: Pierre-Nicholas Roy, University of Waterloo

*“Path integral approaches to study molecular systems at low temperature: Rotations, exchange, and other challenges.”*

2:45–3:30 pm: Zlatko Bačić, New York University

*“Hydrogen molecules in nanoscale cavities: Anharmonic translation-rotation eigenstates, inelastic neutron scattering spectroscopy, and a surprising selection rule for H2@C60.”*

3:30–4:00 pm: Coffee Break

     4:00–4:45 pm: Stephen Fitzgerald, Oberlin College

“*Overtone vibrational spectroscopy and anharmonic behavior in adsorbed molecular hydrogen****.”***

4:45–5:30 pm: Yohann Scribano, Université Montpellier

“*A quantum study of the water-hydrogen complex: From dimer to hydrogen clathrate hydrate****.”***

6:00-9.00 pm: Picnic at the AhHa School for the Arts, 300 S. Townsend (Family and guests welcome, free of charge)

**Tuesday, July 15:**

Session III (Afternoon), TSRC

**Chair:** Joel Bowman, Emory University

1:15–2:00 pm: Maria Pilar de Lara-Castells, CSIC Madrid

*“A full-configuration interaction nuclear-orbital approach to small doped 3He clusters and comparison with 4He and para-H2 counterparts.”*

2:00–2:45 pm: Peter Felker, University of California Los Angeles

*“Calculation of translation-rotation states of multiple confined diatomics.”*

2:45–3:15 pm: Coffee Break

     3:15–4:00 pm: Lorenzo Ulivi, CNR, Sesto Fiorentino

“*Neutron and light spectroscopy of nanoconfined light molecules in different H2O crystals****.”***

4:00–4:45: Martin Quack, ETH Zürich

“*Recent results on mode selective intramolecular energy flow and tunneling dynamics from high resolution infrared spectroscopy of polyatomic molecules and clusters****.”***

6:00–7:15 pm: TSRC Town Talk, Conference Center in Mountain Village

Session IV (Evening), TSRC

**Chair:** Marie-Pierre Gaigeot, Université d’Evry

8:00–8:45 pm: Attila Császár, Eötwös Loránd University

*“Rovibrational energy levels of H3+ and H5+.”*

8:45–9:30 pm: Dominik Marx, Ruhr-Universität, Bochum

*“Understanding large-amplitude motion in the gas phase, in aqueous solutions, and in superfluid helium.”*

**Wednesday, July 16:**

Session V (Afternoon), TSRC

**Chair:** Martin Quack, ETH Zürich

1:15–2:00 pm: Tucker Carrington, Queens University

*“Exploiting sum of products structure to compute vibrational spectra without storing full-dimensional vectors.”*

2:00–2:45 pm: Carolin König, Aarhus Universitet

*“Coordinates and couplings for efficient vibrational structure calculations.*

2:45–3:30 pm: David Perry, University of Akron

“*Large-amplitude motion, coupled vibrations, and conical intersections****.”***

3:30–4:00 pm: Coffee Break

     4:00–4:45 pm: Marie-Pierre Gaigeot, Université d’Evry

“*DFT-MD simulations and vibrational spectroscopy****.”***

4:45 –5:30 pm: David Leitner, University of Nevada Reno

“*Vibrational energy transfer across molecular interfaces****.”***

6:00–7:45 pm: Conference dinner at New Sheridan Chop House, 231 W. Colorado Ave. ($55 per person, includes three courses, tip, and tax-free; drinks extra).

Session VI (Evening), TSRC

**Chair:** Claude Leforestier, Université Montpellier

8:00–8:45 pm: Noam Agmon, Hebrew University

*“Infrared spectra of small protonated water clusters.”*

8:45–9:30 pm: Andrei Tokmakoff, University of Chicago

*“The IR spectroscopy of water and aqueous protons.”*

**Thursday, July 17:**

Session VII (Afternoon), TSRC

**Chair:** Noam Agmon, Hebrew University of Jerusalem

2:00–2:45 pm: Ove Christiansen, Aarhus Universitet

*“Mode-mode correlation and anharmonic wave functions: New insights from coupled cluster theory and tensor decomposition.”*

2:45–3:30 pm: Motoyuki Shiga, Japan Atomic Energy Agency

*“Ab initio and QM/MM path integral simulations of hydrogen bonded systems.”*

3:30–4:00 pm: Coffee Break

     4:00–4:45 pm: Wei Zhuang, Dalian Institute for Chemical Physics, CAS

“*Exploring the ionic solution dynamics using the combination of simulation and vibrational spectroscopy****.”***

4:45–5:30 pm: Mark Tuckerman, New York University

“*Connecting solvation shell structure to proton transport kinetics and vibrational spectroscopy in condensed phases using first principles molecular dynamics****.”***

6:00–7:45 pm: Group dinner at Rustico Ristorante, 114 E. Colorado Ave. ($55 per person, includes three courses, tip, and tax-free; drinks extra).

Session VIII (Evening), TSRC

**Chair:**  Maria Pilar de Lara-Castells, CSIC Madrid

8:00–8:45 pm: Lauri Halonen, University of Helsinki

*“Dissociation of acids on the quasi-liquid layer of ice and wet quartz.”*

8:45–9:30 pm: Fabien Gatti, Université Montpellier

*“Applications of the multiconfiguration time-dependent Hartree (MCTDH) method to vibrational problems: Diffusion rates of molecules on metal surfaces, processes guided by laser pulses, and strong isotopologue selectivity of ozone.”*

**Friday, July 18:**

7:30–8:30 am: Breakfast at TSRC.

Session IX (Morning), TSRC

**Chair:** Wei Zhuang, Dalian Institute for Chemical Physics, CAS

8:30–9:15 am: Asaf Shimshovitz, Weizmann Institute of Science

*“Phase-space approach to solving the Schrödinger equation.”*

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

*“Toward thirty-thousand quantum states of benzene.”*

10:00–10:30 am: Coffee Break

     10:30–11:15 am: David Lauvergnat, Université Paris-Sud

“*Quantum dynamics with sparse grids: Application to floppy molecular systems****.”***

11:15 am–12:0 pm: Discussion on future directions.

12:00 pm: END OF THE WORKSHOP