

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

**Telluride Workshop, July 17–21, 2017**

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

**TSRC hosts: Mark Kozak (970) 708-4426, Kristen Redd (970) 729-8375**

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

**Sunday, July 16:**

6:00–8:00 pm: Meet and Greet informal gathering and registration, Phoenix Bean, 220 E Colorado Avenue. Cash bar.

**Monday, July 17:**

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:** Zlatko Bačić, New York University (USA)

8:30–9:15 am: Ove Christiansen, Aarhus Universitet (Denmark)

*“Construction of potential energy surfaces: Automatic procedures from small to large molecules.”*

9:15–10:00 am: Deborah Crittenden, University of Canterbury (New Zealand)

*“A transformative approach to constructing potential energy surface expansions.”*

10:00–10:30 am: Coffee Break

10:30–11:15 am: David Perry, University of Akron (USA)

*“A Jahn-Teller Hamiltonian for large-amplitude motion on a Sphere in  $E \otimes e$  and  $T_2 \otimes e$  systems: applications to vibrational conical intersections.”*

11:15 am –12:00 pm: Group Discussion

12:00–2:00 pm: Lunch, on your own.

Session II (Afternoon), TSRC

**Chair:** Hans-Dieter Meyer, Universität Heidelberg (Germany)

2:00–2:45 pm: Tucker Carrington, Queens University (Canada)

*“Two ideas for exploiting sum-of-products structure to compute a vibrational spectrum: beyond ten atoms.”*

2:45–3:30 pm: Henrik Larsson, Universität Kiel (Germany)

*“Dynamical pruning in phase, position and configuration space: Efficient approaches for multidimensional quantum dynamics.”*

3:30–4:00 pm: Coffee Break

4:00–4:45 pm: Bill Poirier, Texas Tech University (USA)

*“Rovibrational states for free: The J-dependent rotational Hamiltonian method.”*

4:45–5:30 pm: Ryan Steele, University of Utah (USA)

*“Exploiting locality for anharmonic vibrational spectroscopy simulations.”*

5:30 – 6:00 pm: Group Discussion

**Tuesday, July 18:**

Session III (Afternoon), TSRC

**Chair:** Mark Tuckerman, New York University (USA)

1:15–2:00 pm: Stuart Althorpe, University of Cambridge (UK)

*“Path-integral simulations of tunneling splittings in water clusters.”*

2:00–2:45 pm: Hans-Dieter Meyer, Universität Heidelberg (Germany)

*“Infrared absorption spectrum of the hydrated hydroxide ( $H_3O_2^-$ ) cluster anion. Comparison with the experimental Ar vibrational pre-dissociation spectrum.”*

2:45–3:15 pm: Coffee Break

3:15–4:00 pm: Pushp Bajaj, University of California San Diego (USA)

*“Spectroscopic investigation of halide-hydration in small clusters.”*

4:00–4:45 pm: Martin Suhm, Georg-August Universität Göttingen (Germany)

*“How much anharmonicity in small hydrogen bond shifts and splittings? Benchmarking experiments!”*

4:45 – 5:15 pm: Group Discussion

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

Session IV (Evening), TSRC

**Chair:** Shinichi Miura, Kanazawa University (Japan)

8:00–8:45 pm: Attila Császár, Eötvös Loránd University (Hungary)

*“The chemical fairyland of loosely bound molecules.”*

8:45–9:30 pm: Fabien Gatti, Université de Montpellier (France)

*“Multidimensional quantum mechanical treatment of electron transfer in plant cryptochrome and of the control of the ring opening in spiropyrane molecules.”*

9:30 – 10:00 pm Group Discussion

**Wednesday, July 19:**

7:30–8:15 am: Breakfast at TSRC

Session V (Morning), TSRC

**Chair:** Tucker Carrington, Queens University (Canada)

8:30–9:15 am: Joshua Baraban, University of Colorado Boulder (USA)

*“Spectroscopic signatures of isomerization.”*

9:15–10:00 am: Uve Manthe, Universität Bielefeld (Germany)

*“Ro-vibrational quantum states of fluxional systems.”*

10:00–10:30 am: Coffee Break

10:30–11:15 am: Martin Quack, ETH Zürich (Switzerland)

*“Molecules in motion: Quantum dynamics of chiral and achiral molecules and clusters including parity violation, tunneling and electromagnetic fields.”*

11:15 –11:45 am: Group Discussion

11:45 am –1:15 pm: Lunch, on your own.

Session VI (Afternoon), TSRC

**Chair:** Deborah Crittenden, University of Canterbury (New Zealand)

1:15–2:00 pm: Shinichi Miura, Kanazawa University (Japan)

*“Quantum structural fluctuation in small and medium-sized para-hydrogen clusters.”*

2:00–2:45 pm: Mark Tuckerman, New York University (USA)

*“Hydrogen diffusion and lithium isotope fractionation: Cases of competing and (sometimes) surprising quantum effects.”*

2:45–3:30 pm: Sophya Garaschuk, University of South Carolina (USA)

*“Nuclear quantum effects of the H/D substitution on properties of materials.”*

3:30–4:00 pm: Coffee Break

4:00–4:45 pm: Jian Liu, Peking University (China)

*“Anharmonic effects in the vibrational spectroscopy: Quantum simulations of gas-phase molecules and condensed-phase systems.”*

4:45–5:30 pm: Yohann Scribano, Université de Montpellier (France)

*“A Smolyak sparse-grid scheme for the quantum dynamics of confined molecular hydrogen.”*

6:00–8:00 pm: Picnic

**Thursday, July 20:**

Session VII (Afternoon), TSRC

**Chair:** Jian Liu, Peking University (China)

2:00–2:45 pm: Zlatko Bačić, New York University (USA)

*“On the origin of the symmetry breaking in  $H_2@C_{60}$  and quantum translation-rotation dynamics of  $(H_2O@C_{60})_n$  ( $n=1,2$ ).”*

2:45–3:30 pm: Anthony Horsewill, University of Nottingham (UK)

*“Symmetry breaking in the endofullerene  $H_2O@C_{60}$  revealed in the quantum translation-rotation dynamics of ortho- and para-water studied by neutron scattering.”*

3:30–4:00 pm: Coffee Break

4:00–4:45 pm: Peter Felker, University of California Los Angeles (USA)

*“Electric dipole-dipole coupling in close-packed assemblies of  $H_2O@C_{60}$ .”*

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

*“Quantum statistical mechanics of confined molecules.”*

5:30 – 6:00 pm: Group Discussion

7:00–9:00 pm: Symposium dinner. Partial support by the Canadian Association of Theoretical Chemists is gratefully acknowledged.

### **Friday, July 21:**

7:30–8:30 am: Breakfast at TSRC.

#### Session VIII (Morning), TSRC

**Chair:** Sophya Garaschuk, University of South Carolina (USA)

8:30–9:15 am: Jiri Vanicek, EPFL (Switzerland)

*“On-the-fly ab initio semiclassical evaluation of vibrationally resolved electronic spectra.”*

9:15–10:00 am: Edwin Sibert, University of Wisconsin Madison (USA)

*“CH stretches and the fabulous tail of the alkylbenzenes.”*

10:00–10:30 am: Coffee Break

10:30–11:15 am: Vladimir Mandelshtam, University of California Irvine (USA)

*“Quantum melting and isotope effects from diffusion Monte Carlo studies of para- $H_2$  clusters.”*

11:15 am–12:00 pm: Discussion on future directions.

12:00 pm: END OF THE WORKSHOP