Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems

Telluride Workshop, June 9-14, 2019

Organizers: Zlatko Bačić, Tucker Carrington, Mark Tuckerman

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

Sunday, June 9:

6:00-7:30 PM: Registration and informal gathering at Phoenix Bean, 221 W. Colorado Avenue.

Monday, June 10:

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


9:15–10:00 AM  Gunnar Schmitz: Machine Learning for Potential Energy Surface Construction: More of the same?

10:00–10:30 AM  Coffee Break

10:30–11:15 AM  Justin Talbot: Spectroscopic studies of hydrogen-bonding complexes using eigensolver methodologies

11:15 AM –12:00 PM  Group Discussion

12:00–2:00 PM  Group Catered Lunch at TSRC
Session II (Afternoon), TSRC

**Chair:** Pierre-Nicholas Roy

2:00–2:45 PM Bryan Changala: *Curvilinear mean field-based techniques for spectroscopy, kinetics, and thermodynamics of highly anharmonic molecules*

2:45–3:30 PM Henrik Larsson: *Applying tensor network states to electronic and vibrational systems*

3:30–4:00 PM Coffee Break

4:00–4:45 PM Peter Felker: *Quantum dynamics of light molecules inside fullerenes: Translation-rotation eigenstates, spectroscopy, and symmetry breaking*

4:45–5:30 PM Group Discussion

Tuesday, June 11:

Session III (Afternoon), TSRC

**Chair:** Attila Csaszar

2:00–2:45 PM Zlatko Bačić: *Accurate and efficient full-dimensional quantum calculations of the vibrational eigenstates of weakly bound molecular dimers*

2:45–3:30 PM Ned Sibert: *Large amplitude motions and zero-point effects in the water-benzene complex: Modelling the OH stretch region of the IR spectrum*

3:30–4:00 PM Coffee Break

4:00–5:00 PM Martin Suhm and Armand Nejad: *Formic Acid and its dimer: Let’s BENCH again*

6:30–7:30 PM TSRC Town Talk, Conference Center in Mountain Village, Brian Rubin of the Cleveland Clinic. A cash bar opens at 6:00 PM.
Wednesday, June 12:

7:30–8:15 AM  Breakfast at TSRC

Session IV (Morning), TSRC

Chair:  Ned Sibert

8:30–9:15 AM  Fabien Gatti: About the use of polyspherical coordinates for motions of large amplitude: several recent examples

9:15–10:00 AM  Tucker Carrington: Solving the Schroedinger equation without the variational method: no integrals

10:00–10:30 AM  Coffee Break

10:30–11:15 AM  Sandra Brown: Development of accurate potential energy functions by way of the many-body expansion, with applications to ion-water systems and small organic molecules

11:15–11:45 AM  Group Discussion

11:45 AM – 1:15 PM  Lunch, on your own.

Session V (Afternoon), TSRC

Chair:  Oriol Vendrell

1:15–2:00 PM  Attila Csaszar: Quasistructural molecules

2:00–2:45 PM  Yohann Scribano: Sparse grid methods for high dimensional quantum molecular dynamics with large amplitude motions

2:45–3:30 PM  Pierre-Nicholas Roy: Quantum molecular dynamics of confined molecules

3:30–4:00 PM  Coffee Break

4:00–4:45 PM  Markus Schroeder: Transforming high-dimensional potential energy surfaces into CANDECOMP form using Monte-Carlo methods

4:45–5:30 PM  Jiri Vanicek: Single Hessian thawed Gaussian approximation

6 PM  Picnic, tent behind the school. Open to all TSRC participants, their families, and friends.
Thursday, June 13:

Session VI (Afternoon), TSRC

Chair: Jiri Vanicek

2:00–2:45 PM  Alex Brown: Potential energy surfaces for use in MCTDH

2:45–3:30 PM  Oriol Vendrell: Application of the multi-dimensional time-dependent Hartree approach to highly correlated vibrational and electronic dynamics

3:30–4:00 PM  Coffee Break

4:00–4:45 PM  David M. Benoit: Reviving ab-initio diffusion Monte Carlo

7:00 PM  Symposium dinner at Floradora Saloon, 103 W. Colorado Ave.

Friday, June 14:

7:30–8:15 AM  Breakfast at TSRC.

Session VII (Morning), TSRC

Chair: Tucker Carrington

8:30–9:15 AM  Ehud Pines: New insights on proton solvation and proton transport in water by probing protonated water in acetonitrile

9:15–10:00 AM  Vladimir Mandelshtam: Magic numbers, quantum delocalization and orientational disordering in anionic hydrogen and deuterium clusters

10:00–10:15 AM  Coffee Break

10:15–11:00 AM  Discussion on future directions.

11:00 AM  END OF THE WORKSHOP