Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems

Telluride Workshop, June 9-14, 2019

Organizers: Zlatko Bačić, Tucker Carrington, Mark Tuckerman

TSRC contact: Mark Kozak (970) 708-4426 (mark@telluridescience.org)

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

8:30–9:15 AM Bill Poirier: *The crystal algorithm: Finding – and fixing – leaky "holes" in potential energy surfaces*

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