Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems

Telluride Workshop, June 10-14, 2024

Organizers: Zlatko Bačić and Tucker Carrington

TSRC hosts: Mark Kozak (970) 708-4426, Cindy Fusting (970) 708-5069

Meeting location: Telluride Intermediate School at 721 W. Colorado Ave.

Sunday, June 9:

5:00–6:30 pm: All-Telluride Science Meet and Greet informal gathering and registration, Alibi, 157 S. Fir Street.

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: Joseph Lawrence

8:30–9:15 AM **Attila Császár**

MARVEL, SNAPS, and Hubs

9:15–10:00 AM **Krzysztof Szalewicz**

Breaking 1 cm^{-1} barrier in predictions of spectra of van der Waals clusters

10:00–10:30 AM Coffee Break

10:30–11:15 AM **Tucker Carrington**

Using collocation to solve the vibrational Schrödinger equation

11:15 AM –12:00 PM **Pierre-Nicholas Roy**

Using a discrete variable representation and Gibbs sampling for path integral simulations of interacting rotors

6:00 -8:00 PM: Group dinner in Telluride Science Tent

Session II (**Evening**), TSRC

Chair: Patricia Vindel-Zandbergen

8:30–9:15 PM **Bill Poirier**

Plumbing potentials for molecules with up to tens of atoms: How to find saddle points , fix leaky holes, build hole-free PESs, and find CI seam minima

9:15-10:00 PM **Joseph Lawrence**

Improving the accuracy of instanton theory: pushing the asymptotics

Tuesday, June 11:

Session III (**Afternoon**), TSRC

Chair: David Menedive-Tapia

2:00–2:45 PM **Fabien Gatti**

Quantum dynamics of atoms and molecules on surfaces: CH_4/Ni (13D), H/Graphene (72D)

2:45–3:30 PM **Zlatko Bačić**

Hydrogen-bonded trimers of diatomic molecules: Vibrational states from fully coupled 12D quantum calculations employing contracted intra- and intermolecular bases

3:30–4:00 PM Coffee Break

4:00–4:45 PM **Oriol Vendrell**

High-dimensional quantum dynamics with the ML-MCTDH method: recent developments and applications

4:45 – 5:30 PM **Yohann Scribano**

Role of non-additive three-body interactions in quantum calculations of the coupled vibration-translation-rotation eigenstates of a hydrogen molecule inside clathrate hydrates

6:30–7:30 PM TSRC Town Talk, Conference Center in Mountain Village

Session IV (**Evening**), TSRC

Chair: Rhiannon Zarotiadis

8:30–9:15 PM **Henrik Larsson**

Simulating vibrational spectra of fluxional molecules using tensor network states

9:15–10:00 PM **Hannes Hoppe**

Eigenstates & thermal rate constant calculations in the MCTDH framework

Wednesday, June 12:

7:30–8:15 AM Breakfast at TSRC

Session V (**Morning**), TSRC

Chair: Nore Stolte

8:30–9:15 AM **Jian Liu**

Nonadiabatic field

9:15–10:00 AM **Peter Felker**

Calculation of intermolecular states in water trimer

10:00–10:30 AM Coffee Break

10:30–11:15 AM **Jeremy Richardson**

Path-integral methods for tunneling, geometric phases and exchange of indistinguishable particles

11:15 –12:00 PM **Patricia Vindel-Zandbergen**

Intermolecular rovibrational states of the H_2O-HCN and H_2O-HNC complexes: Insights from new potential energy surface and rigorous quantum calculations

12:00-12:45 PM **Martin Quack** *Title TBA*

5:30–7:30 PM PICNIC. Open to all TSRC participants, their families, and friends.

Thursday, June 13:

Session VI (**Afternoon**), TSRC

Chair: Hannes Hoppe

2:00–2:45 PM **David Lauvergnat**

A new set of coordinates for describing reactive collision processes: Evaluation of the cumulative reaction probability on test cases

2:45–3:30 PM **Jiri Vanicek**

Family of Gaussian wavepacket dynamics methods from the perspective of a nonlinear Schrödinger equation

3:30–4:00 PM Coffee Break

4:00–4:45 PM **David Mendive-Tapia**

Efficient quantum dynamics via deep laddered architectures of the wavefunction

4:45–5:30 PM **Irén Simkó**

HCl trimer: inter- and intramolecular vibrational states from fully coupled 12D quantum calculations

Friday, June 14:

7:30–8:30 AM Breakfast at TSRC.

Session VII (**Morning**), TSRC

Chair: **Irén Simkó**

8:30–9:15 AM **Nore Stolte**

Isotope effects in liquid water at CCSD(T) accuracy with coupled cluster molecular dynamics

9:15–10:00 AM **Rhiannon Zarotiadis**

Nonadiabatic theories of (quantum) nuclear dynamics

10:00–10:30 AM Coffee Break

10:30–11:15 AM **Martin Suhm**

Anharmonic resonances in hydrogen-bonded water molecules and how to tune them experimentally

11:15 AM–12:00 PM Discussion on future directions.

12:00 PM END OF THE WORKSHOP