Spectroscopy and Dynamics of Coupled Anharmonic Vibrations of Floppy Molecular Systems

Telluride Workshop, June 6-10, 2022

Organizers: Zlatko Bačić, Tucker Carrington, Mark Tuckerman

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

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

Sunday, June 5:

5:00–6:30 pm: Meet and Greet informal gathering and registration, Phoenix Bean, 221 W Colorado Avenue. Cash bar.

Monday, June 6:

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 Mark Tuckerman

An exact open-chain path integral distribution for the calculation of quantum time correlation functions

9:15–10:00 AM Henrik Larsson

Tensor network states for simulating fluxional molecular systems

10:00–10:30 AM Coffee Break

10:30–11:15 AM Christoph Schran

Insight into floppy molecular systems from highly accurate neural network representations

11:15 AM –12:00 PM Arman Nejad

Pushing the limits of nuclear structure calculations: Recent advances in the experimental vibrational spectroscopy of formic acid and its dimer

12:00–2:00 PM: Lunch, on your own.

Session II (Afternoon), TSRC

Chair: Tucker Carrington

2:00–2:45 PM Peter Felker

A contracted-basis approach to calculating the intermolecular vibrational states of HF trimer

2:45–3:30 PM Ryan Steele (Virtual)

New, local-mode approaches for anharmonic spectroscopy simulations

3:30–4:00 PM Coffee Break

4:00–4:45 PM Vladimir Mandelshtam

Magic numbers versus quantum delocalization and disordering in neutral and anionic hydrogen clusters

4:45–5:30 PM Markus Schroeder

The coupling of the hydrated proton to its first solvation shell in the Eigen cation

5:30 – 6:00 PM: Group Discussion

Session III (Evening), TSRC

Chair: Markus Schroeder

8:30–9:15 PM Xiang Sun

Photoinduced charge transfer dynamics in the condensed phase

9:15-10:00 PM Jian Liu (Virtual)

Phase space mapping theory for nonadiabatic molecular dynamics

10:00 – 10:30 PM Group Discussion

Tuesday, June 7:

Session IV (Afternoon), TSRC

Chair: Christoph Schran

2:00–2:45 PM Zlatko Bačić

H_2O inside C_{60}: Intra- and intermolecular vibrational states of the guest molecule from fully coupled nine-dimensional quantum calculations

2:45–3:30 PM Pierre-Nicholas Roy

Simulation of entangled confined molecules: from path integrals to matrix product states

3:30–4:00 PM Coffee Break

4:00–4:45 PM David Lauvergnat

A Smolyak algorithm adapted to a system-bath separation: application to an encapsulated molecule with large amplitude motions

4:45 – 5:15 PM Group Discussion

6:30–7:30 PM TSRC TOWN TALK, Conference Center in Mountain Village

Session V (Evening), TSRC

Chair: Arman Nejad

8:30–9:15 PM Jun Li (Virtual)

Data quality, data sampling and data fitting for developing full-dimensional accurate potential energy surfaces of molecular systems

9:15–10:00 PM William Glover (Virtual)

Pushing boundaries: Nonadiabatic dynamics simulations of solvent-supported electronic states

10:00--10:30 PM Group Discussion

Wednesday, June 8:

7:30–8:15 AM Breakfast at TSRC

Session VI (Morning), TSRC

Chair: David Mendive-Tapia

8:30–9:15 AM Nadine Halberstadt (Virtual)

Real time dynamics of dopants in superfluid helium nanodroplets

9:15–10:00 AM Stuart Althorpe (Virtual)

Path-integral dynamics methods for simulating infrared spectra: strengths and weaknesses

10:00–10:30 AM Coffee Break

10:30–11:15 AM Tucker Carrington

A contracted-basis calculation of vibrational levels of water dimer with monomer stretch excitation and a new rectangular collocation method

11:15 –12:00 PM Marko Cvitas

Instanton pathways to vibrational tunneling spectra

12:00–12:30 PM Group Discussion

6:00–8:00 PM PICNIC. Open to all TSRC participants, their families, and friends

Thursday, June 9:

Session VII (Afternoon), TSRC

Chair: Marko Cvitas

2:00–2:45 PM Fabien Gatti

Deciphering the infrared spectrum of the water dimer in the 3500-3800 cm^{-1} energy domain and following vibrations of CO_2 with attosecond pulses

2:45–3:30 PM Yohann Scribano

Smolyak representations with absorbing boundary conditions for reaction path Hamiltonian of reactive scattering

3:30–4:00 PM Coffee Break

4:00–4:45 PM Hannes Hoppe

First-principles theory for the reaction of chlorine with methane

4:45–5:30 PM David Mendive-Tapia

Combining coordinates optimally in protonated floppy molecules for spectroscopy and dynamics with the Multi-Configuration Time-Dependent Hartree (MCTDH) method

5:30 – 6:00 PM Group Discussion

7:00–9:00 pm: Symposium dinner, venue TBD

Friday, June 10:

7:30–8:30 AM Breakfast at TSRC.

Session VIII (Morning), TSRC

Chair: **Mark Tuckerman**

8:30–9:15 AM Bill Poirier

Hitting the Trifecta: How to simultaneously push the limits of Schroedinger solution with respect to system size, convergence accuracy, and number of computed states"

9:15–10:00 AM Roman Ellerbrock

The nonhierarchical correlation discrete variable representation: a quadrature scheme for tree tensor network states

10:00–10:30 AM Coffee Break

10:30–11:15 AM Jiri Vanicek

Capturing finite-temperature effects on vibrationally resolved electronic spectra with ab initio thermo-field Gaussian wavepacket dynamics

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

12:00 PM END OF THE WORKSHOP