Simons Center
International Workshop on Nuclear Quantum Effects in Chemistry

June 12-14, 2023

Monday, June 12: Invited Talks

8:15 am	Continental Breakfast
Session I	**Zlatko Bačić, New York University, Chair**
8:45 am	Welcoming Remarks
9:00 am	Dominik Marx, Ruhr-Universitat Bochum, Germany *Coupled Cluster Path Integrals: From Finite Clusters to the Liquid Phase via Machine Learning*
9:45 am	Sharon Hammes-Schiffer, Yale University *Integrating Electronic and Nuclear Quantum Effects via the Nuclear-Electronic Orbital Approach*
10:30 am	Break
11:00 am	Stuart Althorpe, University of Cambridge, UK *Path-integral dynamics: strengths and weaknesses*
11:45 am	Nancy Makri, University of Illinois at Urbana-Champaign *Real-time path integral methods for including nuclear quantum effects in condensed-phase dynamics*
12:30 pm	Tucker Carrington, Queen's University, Canada *Computing excited OH stretch states of water dimer in 12-D using contracted intermolecular and intramolecular basis functions*
1:15 pm	Lunch and Poster Session

Session II	**Mark Tuckerman, New York University, Chair**
3:00 pm	Zlatko Bačić, New York University *Noncovalently bound molecular dimers and trimers: Full-dimensional quantum calculations of rovibrational states using contracted bases of intermolecular and intramolecular eigenstates*
3:45 pm	Anne McCoy, University of Washington *Using Vibrational Perturbation Theory to Explore Nuclear Quantum Effects*
4:30 pm	Break
5:00 pm	Fabien Gatti, University Paris-Saclay, France *Quantum Dynamics with motions of large amplitude*
5:45 pm	Pierre-Nicholas Roy *Representing entangled molecules using path integrals and matrix product states*
6:30 pm	Conclusion, Day 1

Poster Session
Monday, June 12, 1:15 - 2:45 pm
Hemmerdinger Hall

Author(s)	Institution	Poster Title
Pinchen Xie	Princeton University	*First-principles path-integral molecular dynamics study of ferroelectricity and isotope effects in KDP crystals with deep neural networks*
Davide Moscato	Università degli Studi di Milano	*From anharmonicity to Nuclear Quantum Effects in medium and large sized molecular systems*
Mathew Chow, Tao E. Li, and Sharon Hammes-Schiffer	Yale University	*Building a Condensed Phase Description within Nuclear-Electronic Orbital Dynamics*
Zhou Lin	University of Massachusetts Amherst	*Quantum Mechanical and Machine Learning Modeling of Spectroscopy, Materials, and Catalysis*
Shreyas Malpathak	Cornell University	*Mixed Semiclassical Dynamics: Application to zero-point energy leakage*
Joseph Dickinson	Yale University	*Describing Proton Transfer and Hydrogen Tunneling Dynamics with Nuclear-Electronic Orbital Multistate Density Functional Theory*
Lauren Cook	University College London	*Which Algorithm Best Simulates Nonadiabatic Dynamics Using the Meyer-Miller-Stock-Thoss Hamiltonian?*
Petra Shih	Columbia University	Anharmonic lattice dynamics from vibrational dynamical mean field theory
Henry K. Tran	Columbia University	*Anharmonic Vibrational Spectral Functions using Vibrational Heat-Bath Configuration Interaction*
Dipti Jasrasaria	Columbia University	*Low thermal conductivities of clathrates explained by vibrational dynamical mean-field theory*
George Trenins and Joseph E. Lawrence	ETH Zurich	*New Path-Integral Methods for Accurate Tunneling Splittings*
Xuezhi Bian	University of Pennsylvania	*Modeling spin-dependent chemical dynamics: The role of Berry curvature*

Tuesday, June 13: Invited Talks

8:30 am	Continental Breakfast
Session III	**Tucker Carrington, Queen's University, Chair**
9:00 am	Thomas Markland, Stanford University *Nuclear quantum effects in 3rd order response spectroscopies in the condensed phase*
9:45 am	Mark Tuckerman, New York University *Exact and approximate formulations of single- and two-state quantum time correlation functions in terms of an open-chain path integral distribution*
10:30 am	Break
11:00 am	Jeremy Richardson, ETH-Zurich, Switzerland *A mapping approach to surface hopping*
11:45 am	Joseph Subotnik, University of Pennsylvania *Nonadiabatic Effects at Surfaces and in Solution*
12:30 pm	Timothy Berkelbach, Columbia University *Nuclear quantum effects in anharmonic solids with dynamical mean-field theory*
1:15 pm	Lunch
2:00 pm	Free Time

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Wednesday, June 13: Contributed Talks

8:30 am	Continental Breakfast
Session IV	**Patricia Vindel Zandbergen, NYU, Chair**
9:00 am	Michael Chen, New York University *Machine learning potentials from transfer learning of periodic correlated electronic structure methods: Application to liquid water with AFQMC, CCSD, and CCSD(T)*
9:20 am	Jonathan Fetherolf, Yale University *Capturing electron-proton correlation with multicomponent orbital-optimized perturbation theory*
9:40 am	Chris Haggard, University of Cambridge, UK *Approximations to Matsubara Dynamics for IR Spectra*
10:00 am	Break
Session V	**Irén Simkó, NYU, Chair**
10:20 am	Sohang Kundu, Univ of Illinois at Urbana-Champaign *Quantum Motion of Nuclei Enable the Energy Efficiency of the Bacterial LH2 Complex*
10:40 am	Jinggang Lan, New York University *Uncovering Novel Mechanisms with Nuclear Quantum Effects*
11:00 am	Joseph Lawrence, ETH-Zurich, Switzerland *Moving beyond the instanton: real time paths and state-to-state reaction rates*
11:20 am	Break
Session VI	**Jinggang Lan, NYU, Chair**
11:40 am	Tao Li, Yale University *Quantum Nuclear-Electronic Orbital Dynamics of Plasmon-Driven H2 Catalysis*
Noon	Christopher Malbon, Yale University *Describing Nuclear Quantum Effects with Nuclear-Electronic Orbital Multireference Configuration Interaction*
12:20 pm	Johan Runeson, University of Oxford, UK *Nuclear quantum effects in nonadiabatic dynamics*
12:40 pm	Lunch
Session VII	**Michael Chen, NYU, Chair**
2:00 pm	Tobias Serwatka, University of Waterloo, Canada *Entangled phases in molecular dipolar lattices: A DMRG study*
2:20 pm	Irén Simkó, New York University *On the structure of CH5+ from nuclear density and from the quantum graph model*
2:40 pm	George Trenins, ETH-Zurich, Switzerland *Reaction rates beyond the golden-rule instanton: an interplay of tunnelling and nonadiabaticity*
3:00 pm	Break
Session VIII	**Joseph Lawrence, ETH-Zurich, Chair**
3:20 pm	Patricia Vindel Zandbergen, New York University *Rigorous quantum calculations of rovibrational states of fluxional molecular complexes*
3:40 pm	Robert Wodraszka, Queen's University, Canada *Obviating the need for as many points as basis functions when using collocation with MCTDH to do efficient and accurate quantum dynamics on a general PS*
4:00 pm	Tao (Coraline) Zhen, University of Pennsylvania *Including Berry Force in ab initio Dynamics with Spin-Orbital Coupling*
4:20 pm	Conclusion, Day 3