FUDAN UNIVERSITY

CECAM-BJ

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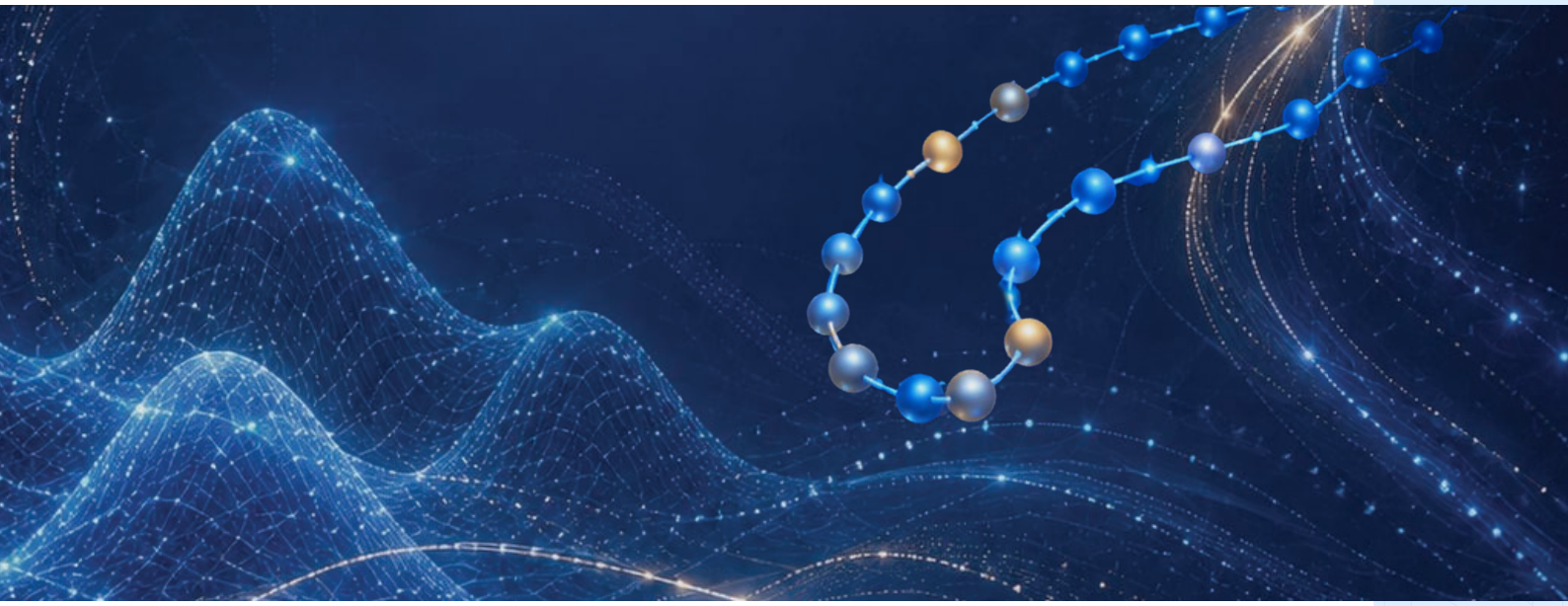
Centre Européen de Calcul Atomique et Moléculaire

Department of Chemistry
100th Anniversary

Path Integral Quantum Mechanics in the Era of Machine Learning

Conference Handbook



July 19–23, 2026

Fudan University

Shanghai, China

Release Date: July 22, 2026

Contents

ABOUT PIQM 2026

The school focuses on molecular simulations based on the path integral formulation of quantum mechanics, which relies on the isomorphism between the partition function of a quantum system and a fictitious classical system of ring polymers. Since the early pioneering work on Path Integral Molecular Dynamics and Monte Carlo, significant progress has been made, e.g., Centroid or Ring Polymer Molecular Dynamics that can approximate quantum response properties such as diffusion coefficients, reaction rates, and spectra. These methods have been applied more widely in recent years, thanks to the development of highly efficient algorithms to include important nuclear quantum effects, such as delocalization, zero-point energy, and tunneling in molecular simulations. Many of them have been implemented in the open-source software i-PI and are used routinely by a global community of computational chemists, physicists, and material scientists, which has grown substantially in the past 15 years.

CECAM has previously supported several advanced Schools (2012, 2016, 2018, 2021, 2023) on path integral quantum mechanics, which helped train a young generation of graduate students and early career researchers in this expanding field. Different from previous events, PIQM 2026 emphasizes path-integral simulations in the context of Machine Learning advancements. The field is currently being revolutionized by algorithms that describe interparticle interactions to significantly accelerate simulations, introducing new paradigms that are potentially reshaping future path-integral methodologies.

DATE: July 19 - 23, 2026
VENUE: Fudan University, Jiangwan Campus
ADDRESS: 2005 Songhu Road, Yangpu District, Shanghai, China
WEBSITE: www.piqm2026.org

ORGANIZING COMMITTEE

Wei Fang
Fudan University

Michele Ceriotti
EPFL

Mariana Rossi
Max Planck Institute
for the Structure and Dynamics
of Matter

Yair Litman
Max Planck Institute
for Polymer Research

Venkat Kapil
University College London

Barak Hirshberg
Tel Aviv University

Thomas Markland
Stanford University

Davide Tisi
EPFL

TOPICS

1 Path Integrals Methods

2 Quantum Rate Theories

3 Semiclassics Methods

4 Machine Learning & Applications

5 Beyond Path Integrals

PROGRAM
Sun July 19, 2026

10:30 – 14:00 Registration

Tutorials

14:00 - 15:00 ***Ab initio* PIMD & Accelerated PIMD**
Michele Ceriotti

15:00 - 15:30 **Path Integral Metadynamics**
Michele Ceriotti

15:30 - 16:00 Coffee break

Tutorials

16:00 - 17:00 **RPMD & CMD**
George Trenins

17:00 - 18:00 **Path Integral Coarse-Graining**
Jing Shen

Conference WiFi

The Wi-Fi is available at the venue during the conference.

SSID: *(to be announced)* Username: **`jqxxsdzdljj`** Password: **`LetsrunPIMD`**

Venue: Linlin Zhou Lecture Hall

PROGRAM
Mon July 20, 2026

8:30 Registration

9:00 - 9:10 **Opening Remarks**

Path Integral Methods Chair: Dong Hui Zhang

9:10 - 9:45 **Economised Path Integrals**
David Manolopoulos

9:45 - 10:20 **Matsubara Dynamics and its Approximations**
Stuart Althorpe

10:20 - 10:50 Coffee break

Path Integral Methods Chair: Mark Tuckerman

10:50 - 11:25 **PIMD Simulations of Bulk Water and Methane Hydrate with Highly Accurate Neural Network Potentials**
Dong Hui Zhang

11:25 - 12:00 **Quantum Dynamics of Hydrogen in Metals and Brownian Chain Molecular Dynamics**
Motoyuki Shiga

12:00 - 13:30 Lunch

Path Integral Methods Chair: David Manolopoulos

13:30 - 14:05 **Paths and Braids: Topological Algorithms for Path Integral Quantum Dynamics**
Mark Tuckerman

14:05 - 14:40 **Fermion Sign Problem and Lee–Yang Phase Transition Theory**
Xin-Zheng Li

14:40 - 15:15 **Bosonic Ring Polymer Molecular Dynamics**
Barak Hirshberg

15:15 - 15:35 **Imaginary Time Path Integral for Fictitious Identical Particles**
Yunuo Xiong

15:35 - 16:05 Coffee break

Tutorials

16:05 - 17:05 **Indistinguishable Particles**
Barak Hirshberg

17:05 - 17:40 **Building your path integral simulations**

18:00 - 21:00 **Poster Session** (with beer & refreshments)

PROGRAM
Tue July 21, 2026

8:30 Registration

Path Integral Methods Chair: Eli Pollak

9:00 - 9:35 **Poissonization of Quantum Dynamics and Applications**
Jiushu Shao

9:35 - 9:55 **Electronic Path-Integral Normal Modes of Mapping Representations for Nonadiabatic Dynamics**
Lauren Cook

9:55 - 10:30 **Exact Tunneling Splittings from Rotationally Projected Path-Integral Sampling**
Yu-Cheng Wang

10:30 - 11:00 Coffee break

Path Integral Methods Chair: Jiushu Shao

11:00 - 11:35 **A Hybrid Quantum Path-Integral Approach to Thermal Correlation Functions**
Nandini Ananth

11:35 - 11:55 **Non-adiabatic Molecular Simulations with Path Integral Monte Carlo**
Michael Hütter

11:55 - 12:30 **Path Integral Methods Session General Discussion**

12:30 - 14:00 Lunch

Semiclassics Chair: Qiang Shi

14:00 - 14:35 **Improving Semiclassical Estimates of Rate Theory and Energy Quantization**
Eli Pollak

14:35 - 15:10 **The Semiclassical Way to Path Integral**
Michele Ceotto

15:10 - 15:45 **Semiclassical Vibronic Spectroscopy with New Initial Value Representation Techniques**
Jia-Xi Zeng

15:45 - 16:15 Coffee break

Semiclassics Chair: Nandini Ananth

16:15 - 16:35 **Herman–Kluk–like Semi-classical Initial-value Representation for Boltzmann Operator**
Peng Zhang

16:35 - 17:10 **Semiclassical Methods for Photoinduced Charge Transfer**
Xiang Sun

17:10 - 17:45 **Semiclassics Session General Discussion**

17:45 - 21:00 **Conference Dinner**

PROGRAM
Wed July 22, 2026

Quantum Rate Theory Chair: Yi Zhao

9:00 - 9:35 **Instanton Theory for Calculating Tunnelling Splittings and Adiabatic Rate Constants**
Marit Fiechter

9:35 - 10:10 **Instanton Theory of Nonadiabatic Tunnelling**
Eric Heller

10:10 - 10:30 **Atomistic Nonadiabatic Reaction Rates from Mean-Field Path Integrals**
Siyu Bu

10:30 - 11:00 Coffee break

Quantum Rate Theory Chair: Yi Zhao

11:00 - 11:20 **A New Path Integral Transition State Theory**
Amira Geuther

11:20 - 11:55 **Memory Matters: Friction in Path-Integral Rate Calculations**
George Trenins

11:55 - 12:30 **Quantum Rate Theory Session General Discussion**

12:30 - 14:00 Lunch

Machine Learning & Applications Chair: Xin-Zheng Li

14:00 - 14:35 **Learning from Experiments with a Quantum Ensemble of Latent Features**
Michele Ceriotti

14:35 - 15:10 **Quantum-State Resolved Dynamics for Complex Reactions Based on Fundamental Invariant-Neural Network (FI-NN) Potential Energy Surfaces**
Bina Fu

15:10 - 15:45 **Applications of PIMD in studying complex aqueous systems**
Jinggang Lan

15:45 - 16:15 Coffee break

Machine Learning & Applications Chair: Michele Ceriotti

16:15 - 16:50 **Machine Learning Potentials at Coupled Cluster Accuracy For Nuclear Quantum Effects In Aqueous Systems**
Christoph Schran

16:50 - 17:25 **Unconventional Superconductivity from Lattice Quantum Disorder**
Yu-Cheng Zhu

17:25 - 17:45 **Quantum Annealing for Materials**
Alfredo Fiorentino

17:45 - 18:05 **Divergence of Semiclassical Expansions: Restoring Spatial Coherence in Density Functional Theory**
Yi Shi

PROGRAM
Thu July 23, 2026

Machine Learning & Applications Chair: Stuart Althorpe

9:00 - 9:35 **How Far Can We Coarse-Grain?**
Zakariya El-Machachi (on behalf of Prof. Cecilia Clementi)

9:35 - 10:10 **Rigorous Quantum Thermodynamics from Entropic Path Integral Coarse-Graining**
Wei Fang

10:10 - 10:45 **Machine Learning & Applications General Discussion**

10:45 - 11:15 Coffee break

Beyond Path Integrals Chair: Michele Ceotto

11:15 - 11:50 **Stochastic Schrödinger Equation for Carrier Dynamics in Organic Semiconductors**
Yi Zhao

11:50 - 12:25 **Memory Kernel Coupling Theory to Quantum Dynamics**
Wenjie Dou

12:30 - 14:00 Lunch

Machine Learning & Applications Chair: Xiao Zheng

14:00 - 14:20 **The Quantum Nature of Non-Equilibrium Proton Transfer — a Full-Wavefunction Dynamics Study**
Luhao Zhang

14:20 - 14:40 **Nuclear Quantum Effects as a Denoising Problem**
Weizhou Wang

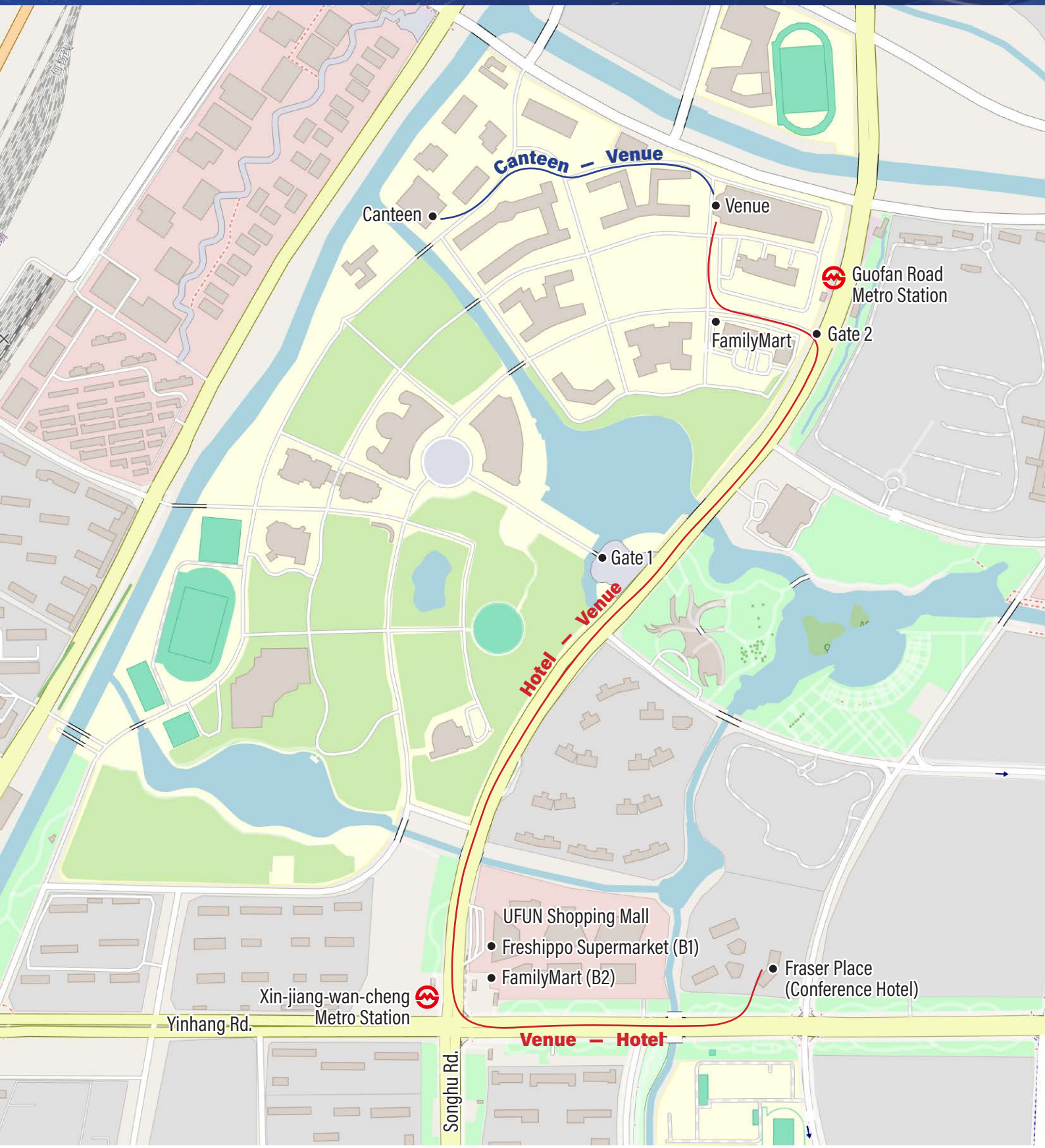
14:40 - 15:15 **Decoding Water from Potentials to Vibrational Spectra**
Qi Yu

15:15 - 15:30 **Ending remarks**

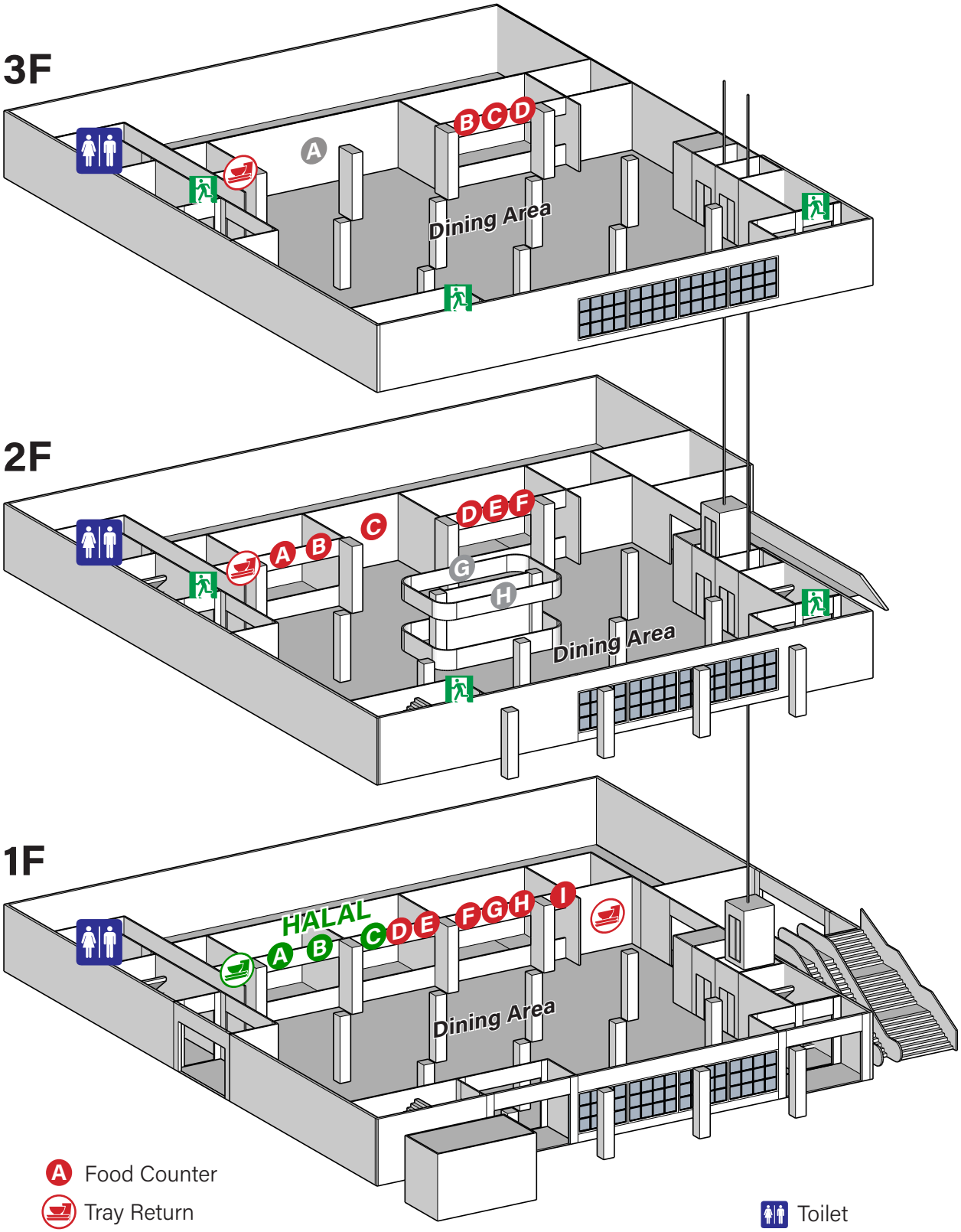
SHUTTLE BUS SCHEDULE

July 19 Sun	**13:30**	Hotel	→	Venue
July 20 Mon	**08:20**	Hotel	→	Venue
July 20 Mon	**17:45**	Venue	→	Hotel
July 21 Tue	**08:30**	Hotel	→	Venue
July 21 Tue	**17:45**	Venue	→	Dinner Venue
July 21 Tue	**21:00**	Dinner Venue	→	Hotel
July 22 Wed	**08:30**	Hotel	→	Venue
July 23 Thu	**08:30**	Hotel	→	Venue

MAP


Canteen – Venue
Canteen
Venue
Guofan Road
Metro Station
FamilyMart
Gate 2
Gate 1
Hotel – Venue
UFUN Shopping Mall
Freshippo Supermarket (B1)
FamilyMart (B2)
Fraser Place
(Conference Hotel)
Xin-jiang-wan-cheng
Metro Station
Yinhang Rd.
Venue – Hotel
Songhu Rd.

CANTEEN



- A Food Counter
- Tray Return
- A Food Counter (Halal)
- Tray Return (Halal)
- A Unavailable Food Counter
- Toilet
- Emergency Exit

CANTEEN

Voucher Instructions

- Lunch will be available at the canteen on all four conference days, July 20–23.
- Each voucher may be used once for purchases of up to RMB 30 at a single food counter.
- Food counters marked in grey do not accept conference vouchers.
- Regular vouchers **cannot** be used at halal food counters.
- Cash, mobile payments, and other forms of payment are not accepted.
- **Vegetarian** and **kosher** meals should be collected on the third floor (3F).

1F

A **Chinese Northwest-Style Fast Food (Halal)**

B **Chinese Northwest-style Stir-Fries (Halal)**

C **Chinese Northwest-style Hand-pulled Noodles (Halal)**

D **Sliced beef tenderloin rice noodles**

E **Sichuan-style Kitchen**

F **Jiangnan Dim Sum**

G **Teppanyaki & Barbecue**

H **Spicy Hot Pot**

I **Specialty Stir-Fries**

2F

A **Iron Pot Braised Noodles**

B **Fast Food**

C **Stir-Fries**

D **Specialties**

E **Cantonese roasted & Marinated delights**

F **Western Casual Meal**

G *Healthy Life (voucher not accepted)*

H *Burgers & Pizza (voucher not accepted)*

3F

A *Pay-by-weight Buffet (voucher not accepted)*

B **Chinese noodles**

C **Topped Rice**

D **Snacks and Sweet soup**

E **Peking Duck**

F **Cold Dishes**

DINING AND DAILY ESSENTIALS

The following nearby stores offer snacks, drinks, packaged food, ready-to-eat meals, and daily necessities. Their approximate locations are marked on the map on page 11.

1 **FamilyMart**

Location: Just inside Gate 2 of Fudan University, Jiangwan Campus.

2 **FamilyMart**

Location: B2 level of UFUN Shopping Mall (B2 level), near metro station.

3 **Freshippo Supermarket**

Location: B1 level of UFUN Shopping Mall.

Vegetarian restaurant option nearby:

1 **Wushu Shangjiao（舞蔬尚饺）**

Vegetarian Chinese Cuisine & Dumplings

Address: 177 Guo'an Road

Halal restaurant options nearby:

1 **KAXKAR Tami（塔米新疆烤肉）**

Halal Xinjiang Cuisine & BBQ

Address: 678 Yinhang Road

2 **Asa（阿萨中东料理）**

Halal Middle Eastern Cuisine

Address: Room 1213, Building C, Wanda Plaza, No. 189 Zhengtong Road

ABSTRACT

Invited Speakers
(alphabetic order)

Matsubara Dynamics and its Approximations

Stuart C. Althorpe

Yusuf Hamied Department of Chemistry, University of Cambridge, Cambridge, UK.

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Matsubara dynamics is the rigorous semiclassical limit underpinning path-integral dynamics methods such as ring-polymer molecular dynamics (RPMD) and centroid molecular dynamics (CMD). This talk will show how Matsubara dynamics arises from exact quantum dynamics by smoothing the imaginary-time Feynman paths (ring polymers). We will be upfront about the practical shortcomings of Matsubara dynamics (it has a massive phase problem that makes it impossible to simulate!) and show how the various practical path-integral methods (RPMD, CMD, QCMD, etc.) approximate Matsubara dynamics by averaging out the phase. If time permits, we will also discuss some recent applications of Matsubara dynamics to quantum rate theory.

[1] Althorpe, S.C. Eur. Phys. J. B, 2021, 94, 155.
[2] Trenins, G.; Willatt, M.J.; Althorpe, S.C. J. Chem. Phys., 2019, 151, 054109.

A Hybrid Quantum Path-Integral Approach to Thermal Correlation Functions

Nandini Ananth

Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY 14853

Real-time thermal correlation functions are challenging to compute for condensed-phase systems. While path-integral Monte Carlo (PIMC) methods have been highly successful in describing the dynamics of low- dimensional systems coupled to dissipative environments, extending these approaches to larger quantum systems is limited by the cost of evaluating short-time propagator matrix elements.

In this talk, I introduce the hybrid Path Integral Monte Carlo (hPIMC) method, which combines classical path-integral sampling with a quantum algorithm for evaluation of the short-time propagator matrix elements [1]. After briefly reviewing the foundations of classical PIMC and quantum simulations on spin-based hardware, I show how we can leverage these ideas to build a hybrid quantum algorithm. The resulting hPIMC algorithm em- ploys Probabilistic Imaginary-Time Evolution (PITE) to treat the imaginary-time component of the propagator and a grid-based Discrete Variable Representation (DVR) approach to simulate kinetic-energy evolution. I dis- cuss the scaling of the method and its application to real-time thermal correlation functions in condensed-phase systems, and show that hPIMC achieves an asymptotic quantum speedup over classical PIMC.

[1] E. Eklund and N. Ananth, Digit. Discov. 5, 2759 (2026).

ABSTRACT

Invited Speakers

The Semiclassical Way to Path Integral

Michele Ceotto

Dipartimento di Chimica, Università degli Studi di Milano, via Golgi 19, 20133, Milano

* michele.ceotto@unimi.it

The semiclassical approximation for the quantum propagator is introduced by approximating the path integral expression. This approximation, called semiclassical initial value representation (SCIVR), is implemented for spectroscopic calculations, [1,2,3] including IR spectra and vibrational eigenfunction representation. Several applications, ranging from gas to gas-surface and liquid phase will be presented. [4,5]

In the second part of the talk the semiclassical approximation is applied to reaction rate constant calculations. Specifically, the semiclassical transition state theory approximation (SCTST) will be recalled. I will show how SCTST can be implemented at CCSD(T) level of electronic structure theory. This implementation allows us to estimate how heavy atoms are affecting tunneling. Then, I will present SCTST condensed phase applications and show that solvent may be a factor in tunneling. [6]

In the third and last part of the talk, I will present a new semiclassical non-adiabatic method based on thawed Gaussian wavepacket dynamics. [7]

[1] R. Conte, G. Mandelli, G. Botti, D. Moscato, C. Lanzi, M. Cazzaniga, C. Aieta, M. Ceotto, *Chem. Sci.* 16, 20-28 (2025);
[2] R. Conte, C. Aieta, M. Cazzaniga, and M. Ceotto, *J. Chem. Phys. Lett.* 15, 7566-7576 (2024);
[3] R. Conte, C. Aieta, M. Ceotto, *Chem. Sci.* 17, 3430-3448 (2026);
[4] E. Fallacara, F. Finocchi, M. Cazzaniga, S. Chenot, S. Stankic, M. Ceotto, *Angew. Chem. Int. Ed.* 63, e202409523 (2024);
[5] D. Moscato, G. Mandelli, M. Bondanza, F. Lipparini, R. Conte, B. Mennucci, M. Ceotto, *J. Am. Chem. Soc.* 146 (12), 8179–8188 (2024);
[6] G. Mandelli, C. Aieta, M. Ceotto, *Chem. Sci.* 17, 448 (2026)
[7] L. Bocchi, J.-X. Zeng, M. Ceotto, *J. Chem. Phys.* (submitted).

Learning from Experiments with a Quantum Ensemble of Latent Features

Michele Ceriotti

Institute of Materials, EPFL

* michele.ceriotti@epfl.ch

Predicting NMR chemical shifts from first principles, and then using the measurements to improve the prediction, is a natural goal for machine learning in the physical sciences, and one that NMR crystallography puts directly to the test.

The standard workflow compares shieldings computed for static structures against experiment, but ignoring the thermal and quantum motion of the nuclei badly distorts the result for hydrogen-bonded protons.

In this talk I'll describe how a learned shielding model represents each structure through a set of latent features, then averages them over a quantum ensemble sampled with a transferable machine-learning potential. This roughly halves the disagreement with experiment for protons, and lets us fine-tune those same features directly against measured shieldings, reducing further the error beyond what can be achieved based on approximate electronic-structure techniques.

How Far Can We Coarse-Grain?

Cecilia Clementi
Freie Universität Berlin
* cecilia.clementi@fu-berlin.de

Coarse-graining is a well-established process for reducing degrees of freedom, making long-timescale and complex many-body simulations tractable. This approach has yielded numerous success stories across varying domain sizes, bridging the gap from modeling biomolecules to density functional theory (DFT). This talk will highlight three specific applications of this philosophy: a transferable coarse-grained model for proteins, the temperature-elevated path integral coarse-grained simulation (Te-PIGS) protocol, and how machine learning interatomic potentials (MLIPs) can account for long-range interactions using global message passing.

Memory Kernel Coupling Theory to Quantum Dynamics

Wenjie Dou
Westlake University

Time correlation functions (TCFs) are fundamental quantities governing transport coefficients, optical spectra, and chemical reaction rates. However, accurately calculating TCFs for complex quantum systems remains a major computational challenge because conventional approaches generally require propagating the full quantum dynamics. We developed Memory Kernel Coupling Theory (MKCT), a new framework for directly computing time correlation functions from higher-order moments. Rather than explicitly propagating projected dynamics, MKCT decomposes the memory kernel into a hierarchy of auxiliary kernels governed by linearly coupled equations. This formulation requires only a single steady-state calculation, making the computational cost largely independent of system size. Benchmark on both bosonic and fermionic open quantum systems demonstrate that MKCT reproduces numerically exact results. Because MKCT is not restricted to Gaussian environments or linear system-bath couplings, it establishes a broadly applicable framework for studying quantum dynamics in realistic systems.

ABSTRACT

Invited Speakers

Rigorous Quantum Thermodynamics from Entropic Path Integral Coarse-Graining

Wei Fang

Department of Chemistry, Fudan University, Shanghai, 200438, P. R. China

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Nuclear quantum effects (NQEs) are essential for isotope effects, tunnelling, and quantum thermodynamics, but their rigorous treatment by imaginary-time path-integral methods remains costly for complex molecular systems. I will present entropic path-integral coarse-graining (EPIGS), a framework that replaces explicit imaginary-time replica sampling with a learned quantum effective potential. The key idea is to encode quantum Boltzmann statistics through the free energy of the path-integral centroid and its derivatives with respect to temperature and nuclear mass, which correspond to centroid entropy and quantum kinetic energy. This is enabled by two advances. First, an instanton-based free-energy perturbation scheme makes these quantities accessible at practical cost. Second, a neural-network architecture treats temperature and nuclear masses as explicit inputs and is trained jointly on the effective potential, entropy, and kinetic energy, enabling temperature- and isotope-transferable quantum effective potentials. Classical MD on EPIGS potentials then yields rigorous quantum thermodynamic properties at near-classical computational cost. Benchmarks on hydrogen-bonded systems, including liquid water, show sub-meV/atom agreement with full path-integral simulations for quantum free energies and enthalpies. EPIGS opens the door to large-scale simulations of NQEs and isotope effects in complex systems that remain beyond routine path-integral simulations.

[1] https://arxiv.org/abs/2602.18821

Instanton Theory for Calculating Tunnelling Splittings and Adiabatic Rate Constants

Marit R. Fiechter

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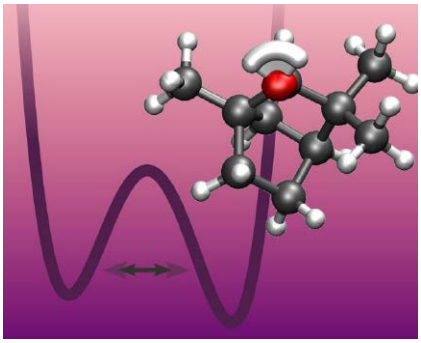
* marit.fiechter@phys.chem.ethz.ch

Instanton theory forms an efficient approximation to path-integral quantum mechanics, and has proven highly useful for capturing quantum nuclear effects in a range of molecular systems. In my talk, I will lay out the basics of instanton theory, with a focus on the calculation of tunnelling splittings and adiabatic reaction rate constants [1]. I will then talk about recent developments, e.g. the extension of tunnelling splitting calculations to asymmetric double-well system [2], tunnelling in strong electric [3] or magnetic fields, and the relation between tunnelling frequencies and rates [2].



[1] Richardson, J. O. *International Reviews in Physical Chemistry*, **2018**, *37*(2), 171–216.
[2] Fiechter, M.R.; Laude, G.; Richardson, J.O. *Journal of Chemical Physics*, **2026**, *164*(12), 124115.
[3] Geuther, J. A.; Fiechter, M. R.; Richardson, J. O. *Molecular Physics*, **2026**, e2636087.

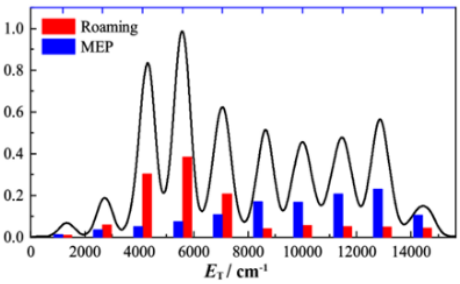
Quantum-State Resolved Dynamics for Complex Reactions Based on Fundamental Invariant-Neural Network (FI-NN) Potential Energy Surfaces

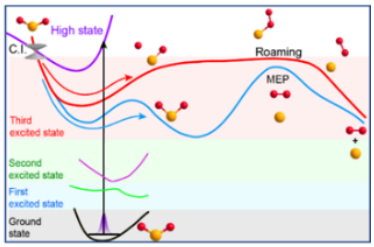
Bina Fu

State Key Laboratory of Chemical Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian

* bina@dicp.ac.cn

State-resolved complex molecular dynamics theory is crucial for understanding phenomena in fields such as interstellar atmospheres and combustion chemistry. However, due to limitations in theoretical methods, high-precision, quantum state-resolved dynamics studies were traditionally confined to systems with low electronic states and a few atoms. We have developed an efficient and accurate Fundamental Invariant-Neural Network (FI-NN) potential energy surface construction method, which has advanced state-resolved dynamics research to reaction systems involving more than 10 atoms. Through excited-state potential energy surface construction and state-resolved dynamics methods, combined with experimental collaboration, we discovered the first roaming mechanism in molecular high-excited-state dissociation, offering a new perspective for understanding and predicting photochemical reactions. Furthermore, we identified unique collision-induced roaming mechanisms in complex molecular reactions, providing theoretical insights for the development and refinement of theoretical models.





[1] Z. Li, Y. Fu, B. Fu*, K. Yuan*, D. H. Zhang, X. Yang, et al. *Science*, 383, 746 (2024).
[2] Y. Liu, L. Liu, B. Fu*, W. Dong*, D. H. Zhang*, X. Yang*, et al. *Nat. Chem.*, 17, 897 (2025).
[3] Y. Bai, Y. Fu, Y. Han, D. H. Zhang et al, B. Fu*, *Nat. Commun.*, 16, 2732 (2025).
[4] B. Fu*, D. H. Zhang*, *Natl. Sci. Rev.*, 10, nwad321 (2023).
[5] L. Liu, Y. Fu, D. H. Zhang et al, B. Fu*. *J. Phys. Chem. Lett.*, 16, 460 (2025).

Bosonic Ring Polymer Molecular Dynamics

Barak Hirshberg

Tel Aviv University

* hirshb@tauex.tau.ac.il

We present a method for approximating real-time correlation functions and quantum transport coefficients of bosonic condensed phases. The direct evaluation of quantum time correlation functions in the path integral formulation is impossible due to a severe dynamical sign problem. Evaluating imaginary-time correlation functions and inverting them using analytic continuation is famously ill-posed. Ring polymer molecular dynamics (RPMD) provides an alternative approach resulting in accurate approximations for real-time correlation functions of condensed phases but neglects exchange effects. In this work, we develop a bosonic RPMD method, which is exact in the harmonic, short time, and high temperature limits. A critical enabling observation is that the Kubo-transformed correlation function for bosons is real only when the correlated observables are symmetric under exchange. We benchmark the method on harmonic and anharmonic model systems and then use it to directly obtain the Lieb-Liniger gas density-density real-time correlation functions at various temperatures and momentum transfers. This work enables the direct simulation of finite-temperature, real-time dynamics of large bosonic condensed phases while accounting for exchange effects for the first time.

ABSTRACT

Invited Speakers

Instanton Theory of Nonadiabatic Tunnelling

Eric R. Heller

Department of Chemistry, University of California, Berkeley, 94720 Berkeley, USA
Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA

Nuclear quantum effects shape many chemical reactions, especially when light atoms such as hydrogen are transferred. Most theoretical studies of such effects rely on the Born–Oppenheimer approximation, assuming that the reaction occurs on a single electronic state. Particularly in photo- and electrochemistry, however, nonadiabatic reactions involving changes in both molecular geometry and electronic state are ubiquitous. While Marcus theory provides a foundational description of nonadiabatic rate processes, its classical treatment of nuclear motion can lead to substantial inaccuracies when molecularscale tunnelling is important. A fully quantum-mechanical treatment of realistic molecular systems, meanwhile, remains computationally infeasible [1].

In this talk, I will present recent progress in the development and application of golden-rule instanton theory: a rigorous semiclassical approximation to the exact path-integral expression for the golden-rule rate [2,3]. The theory predicts tunnelling rates from the optimal imaginary-time path, or instanton, connecting reactant and product electronic states. This provides an intuitive picture of the reaction mechanism in terms of a classical trajectory travelling beneath the potential-energy barrier (see Fig. 1). It will be shown that tunnelling in nonadiabatic reactions can qualitatively change reaction mechanisms and lead to rate enhancements by many orders of magnitude, especially in the inverted regime. This enables room-temperature tunnelling even of heavy atoms such as carbon, nitrogen, and oxygen. The resulting instanton rates agree closely with exact quantum-mechanical benchmarks for model systems, while coupling the method to multireference electronic-structure calculations leads to quantitative agreement with matrix-isolation and laser experiments [4]. Recent extensions of instanton theory to reactions through conical intersections and competing reaction mechanisms further broaden this picture [5]. Together, these developments challenge the common expectation that tunnelling is relevant mainly for hydrogen transfer or cryogenic chemistry, suggesting that heavy-atom tunnelling in nonadiabatic reactions may be far more prevalent than previously anticipated, even under ambient conditions.

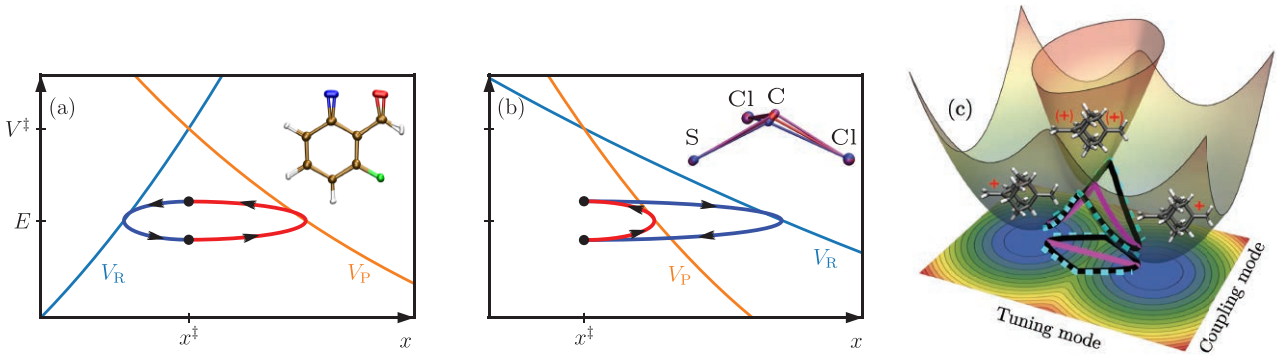


Figure 1: Reactant (V_R) and product (V_P) potentials with instantons in the normal (a) and inverted (b) regimes consisting of one path on each potential (dark colours). The insets show the change of the molecular configuration due to tunnelling along the instantons. (c) Conical intersection mediating a charge transfer, along with several competing instantons.

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Applications of PIMD in Studying Complex Aqueous Systems

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Nuclear quantum effects (NQEs) play an essential role in determining the structure, dynamics, and reactivity of complex aqueous systems. In this talk, I will present recent advances in applying first-principles and machine-learning-accelerated path-integral molecular dynamics (PIMD) to study metal–water interfaces and solvated electrons. These simulations reveal how quantum fluctuations govern hydrogen-bond networks, proton transfer, and spectroscopic signatures beyond the reach of classical molecular dynamics. The combination of PIMD with machine learning has made quantum simulations of realistic aqueous systems computationally practical, providing new insights into electrochemical and solvation phenomena.

Fermion Sign Problem and Lee–Yang Phase Transition Theory

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To simulate indistinguishable particles, recent studies of path-integral molecular dynamics formulated their partition function Z as a recurrence relation involving a variable ξ, with $\xi = 1(-1)$ for bosons (fermions) [1-3]. Inspired by Lee–Yang phase transition theory, we extend ξ into the complex plane and reformulate Z as a polynomial in ξ [4]. By analyzing the distribution of the partition function zeros, we gain insights into the analytical properties of indistinguishable particles, particularly regarding the fermion sign problem (FSP). We found that at 0 K, the partition function zeros for N particles are located at $\xi = -1, -1/2, -1/3, ..., -1/(N - 1)$. This distribution disrupts the analytic continuation of thermodynamic quantities, expressed as functions of ξ and typically performed along $\xi = 1 \rightarrow 1$, whenever the paths intersect these zeros. Moreover, we highlight the zero at $\xi = -1$, which induces an extra term in the free energy of the fermionic systems compared to ones at other $\xi = e^{i\theta}$ values. If a path connects this zero to a bosonic system with identical potential energies, it brings a transition resembling a phase transition. These findings provide a fresh perspective on the successes and challenges of emerging FSP studies based on analytic continuation techniques.

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ABSTRACT

Invited Speakers

Economised Path Integrals

David Manolopoulos

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The Hessian of the ring polymer spring potential in the standard Trotter path integral is a symmetric circulant matrix. Since all such matrices have the same eigenvectors (bead to normal mode transformation vectors), the Trotter path integral is not the only possibility that is consistent with the cyclic permutation and inversion symmetries of the beads of the ring polymer necklace: one is free to change the frequencies of the internal modes while keeping their eigenvectors the same. This freedom can be exploited by optimising the normal mode frequencies to fit the exact ($P \to \infty$) quantum mechanical radii of gyration of harmonic ring polymers with frequencies in the range $0 < \omega < \omega_{max}$, where ω_{max} is the maximum physical frequency of interest. A similar idea has been used recently by Hunt and Althorpe to develop an improved hierarchical equations of motion method for open system quantum dynamics [A. C. Hunt and S. C. Althorpe, *J. Chem. Phys.* **164**, 084113 (2026)], but the details here are somewhat different. The optimisation involves solving a simple least squares problem for the optimum (economised or "eco") internal mode frequencies by nonlinear regression (or "machine learning"). This only has to be done once at the beginning of the calculation and it takes at most a few seconds of computer time. The remainder of the calculation then proceeds in exactly the same way as a Trotter path integral calculation. One can continue to use standard estimators for observables such as the centroid virial kinetic energy estimator, and the method can be used to calculate dynamical properties as well as static properties (for example by replacing PIMD with RPMD). Example applications to hexagonal ice at 100 K show that the convergence of the eco path integral with increasing P is comparable to that of the 4th order Suzuki–Chin path integral, but with purely 2nd order Trotter effort. There is no need to calculate the projected Hessians that arise in the Suzuki–Chin path integral by finite differences, there is no need to develop any new estimators, and once the eco frequencies have been calculated the implementation of the eco path integral boils down to changing a single line of a Trotter path integral code.

Improving Semiclassical Estimates of Rate Theory and Energy Quantization

Eli Pollak

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The two fundaments of semiclassical theory are the semiclassical quantization rule of Brillouin, Wentzel, and Kramers on the one hand, and the semiclassical transmission probability through barriers as put forth by Gamow and Kemble on the other. They have survived almost a century of study and applications, yet both have shortcomings. As shown by Schatz in 1979, the BWK (also known as WKB) rule and its multidimensional generalization (EBK quantization) do not agree with second-order perturbation theory. The Kemble expression predicts that the transmission probability through a barrier is 1/2 whenever the incident energy is at the barrier height. This half point rule is incorrect, as may be seen from analytic solutions for Eckart and square barriers. At high temperatures, thermal reaction rates are typically greater than predicted by most semiclassical theories.

In this talk, I will present a rather simple correction to the semiclassical theory,based on second order vibrational perturbation theory, which answers these challenges. Results will be presented for the collinear hydrogen exchange reaction as well as semiclassical quantization of a non-rotating water molecule. The resulting theories are amenable to on-the-fly computations and do not demand averaging over many trajectories.

Machine Learning Potentials at Coupled Cluster Accuracy for Nuclear Quantum Effects In Aqueous Systems

Christoph Schran
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Predictive simulation of aqueous systems demands two ingredients that are hard to reconcile: an accurate potential energy surface and a faithful treatment of nuclear quantum effects. We describe how machine learning potentials trained towards coupled cluster accuracy allow both to be addressed together across a range of aqueous systems.

We begin with liquid water for which we have recently achieved coupled cluster accuracy while accounting for nuclear quantum effects, before turning to the solvation of ions and to the solvated proton in water.

Taking a deliberately pedagogical view, we also assess approximate path integral dynamics for complex floppy systems to give some recommendations on predicting infrared spectra.

Quantum Dynamics of Hydrogen in Metals and Brownian Chain Molecular Dynamics

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Nuclear quantum effects, such as zero-point motion and tunneling, play an important role in hydrogen dynamics in bulk and surface metals. We have studied hydrogenisotope diffusion using path-integral-based methods, including quantum transitionstate theory (QTST), ring-polymer molecular dynamics (RPMD), and centroid molecular dynamics (CMD) [1-3]. Combined with first-principles calculations and machine-learning potentials, these approaches have enabled the quantitative evaluation of isotope effects and have shown good agreement with experiments.

While RPMD and CMD are useful for describing diffusion dynamics, they have intrinsic difficulties in vibrational dynamics. To overcome this limitation, Brownian chain molecular dynamics (BCMD) was proposed as an approximate quantum dynamics method, in which Newtonian dynamics of the centroid mode is combined with overdamped Brownian dynamics of the non-centroid modes [4]. BCMD has been shown to reproduce hydrogen inelastic neutron scattering (INS) spectra, which are difficult to describe by classical dynamics because they reflect local anharmonic hydrogen vibrations and coupling with metal phonons [5].

Recently, path-integral simulations with machine-learning potentials have been accelerated to the nanosecond time scale [6], opening the way to longer-time simulations of quantum molecular systems. We are also developing a theoretical foundation and an improved numerical algorithm for BCMD, particularly through a quasi-density-operator (QDO) formulation and a multiple-time-step scheme designed to enhance numerical stability.

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ABSTRACT

Invited Speakers

Memory Matters: Friction in Path-Integral Rate Calculations

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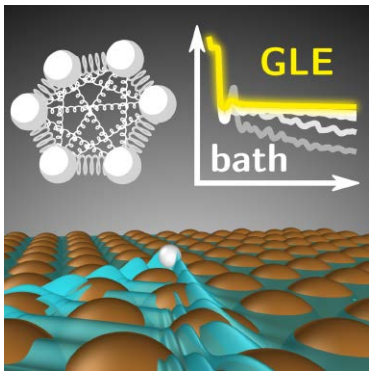
Friction describes how molecular motion is altered by coupling to an "environment", be it solvent, crystalline substrate, or conduction electrons. It can be a key factor in rate calculations: not only does friction control diffusion and energy dissipation, it also modifies quantum zero-point energies and tunnelling probabilities [1,2]. All these effects are captured by ring-polymer generalised Langevin dynamics, which we developed as an extension of RPMD rate theory [3]. We show how the spatial dependence and memory of friction combine to modulate nuclear quantum effects and describe how to incorporate this into practical simulations. Using our approach, we study the diffusion of hydrogen on the Cu(111) surface, finding that memory effects counteract the rate enhancement due to zero-point motion. We show that for a range of temperatures, the two effects cancel almost perfectly, explaining the anomalous agreement of previous classical dynamics simulations with experiment. Outside this range, the diffusion rates display non-Arrhenius behaviour that is not captured by classical dynamics but readily explained by our approach.



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Paths and Braids: Topological Algorithms for Path Integral Quantum Dynamics

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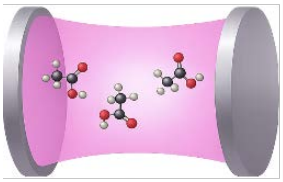

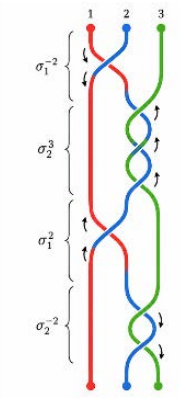

In the path integral formulation of quantum statistical mechanics, imaginary-time paths between two points, which represent general canonical density matrix elements, are often needed for the calculation of momentum-dependent properties, approximate quantum dynamics, and Wigner phase-space functions. In the first part of this talk, I will discuss efficient classical algorithms for the calculation of canonical density matrix elements via open-chain Monte Carlo and open-chain contraction algorithms. The second part of the talk will be an introduction to the, as yet largely unexplored, development of quantum algorithms for path integrals. The discussion will focus specifically on topological quantum algorithms, formulated in terms of the physics of anyons and braiding operations, for computing quantum dynamics. I will review the concepts of anyon fusion in the generation of the computational basis, braid groups, and braiding operations for the construction of quantum gates needed in the calculation of real-time quantum propagators. Simple examples, including isolated small molecules and molecules in optical cavities, as well as system-bath Hamiltonians, will be used to illustrate these concepts and prospects for expanding to larger systems will be presented.

Semiclassical Methods For Photoinduced Charge Transfer

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Simulating photoinduced charge transfer in the condensed phase is essential for understanding fundamental processes in solar energy conversion and complex molecular devices. Traditional approaches, such as standard Marcus theory, often rely on the assumption of a thermally equilibrated initial state. However, this assumption frequently breaks down for photoinduced processes, where vertical excitation creates a highly nonequilibrium nuclear state. The subsequent structural relaxation dictates that the transfer process must be described by a time-dependent rate coefficient. In this talk, I will present semiclassical methods developed to accurately capture these non-stationary dynamics. I will first introduce the nonequilibrium Fermi's golden rule (NE-FGR), which provides a rigorous foundation for evaluating electronic transitions originating from nonequilibrium states. Building upon this framework, I will discuss Instantaneous Marcus Theory (IMT) for photoinduced charge transfer dynamics. By utilizing linearized semiclassical approximations, NE-FGR and IMT successfully captures the time-dependent evolution of charge transfer rates as the system undergoes nuclear relaxation. Furthermore, applying these theories to complex systems requires the construction of accurate model Hamiltonians. To this end, I will discuss the formulation of effective multistate harmonic (MSH) models. Constructed directly from all-atom electronic structure calculations and molecular dynamics simulations, the MSH framework serves as a nontrivial multistate extension of the spin-boson model. I will demonstrate how these MSH models are proven to reproduce the nonadiabatic dynamics of the full all-atom description. Ultimately, the combination of these semiclassical rate theories and MSH model construction offers a robust toolkit for investigating charge and energy transfer dynamics in complex condensed phases.

Poissonization of Quantum Dynamics and Applications

Jiushu Shao
Beijing Normal University

Interpreting the action of the Hamiltonian operator as an event, we demonstrate the correspondence between the quantum dynamics of a generic system and a Poisson process and thereby establish a Poissonization procedure to simulate quantum dynamics. We first clarify the basic ideas of the approach and analyze how the Poisson rate controls the convergence. We then show that the Poissonization naturally results in a quantum jump scheme and make an illustration with the two-state system. For nonadiabatic processes the Poissonization yields an exact stochastic surface hopping approach and we make it clear with the simulation of a Tully's model. Finally, we tackle the Newns-Anderson model with more than a hundred electronic states and obtain the exact vibrational excitation dynamics.

ABSTRACT

Invited Speakers

Exact Tunneling Splittings from Rotationally Projected Path-Integral Sampling

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Quantum tunneling between symmetry-related molecular structures produces characteristic splittings that sensitively probe rovibrational dynamics and the underlying potential energy surface. In this talk, I will present two recent advances in exact path-integral methods for such splittings. First, I will show how the previous symmetrized path-integral molecular dynamics (PIMD) framework for the rotational ground state [1] can be extended to rotationally excited states by projecting onto selected *J* manifolds and symmetry subspaces with an Eckart spring, allowing rigorous rotationally resolved splittings for multiple *J* values to be extracted from a single set of simulations. [2]

In the second part, I will introduce path-integral hybrid Monte Carlo with enveloping bridging potentials (PIHMC-EBP), a new path-integral sampling method based on the same rotational-projection formalism. [3] In this approach, an EBP is constructed for direct free-energy sampling, and two tailored nonlocal updates are designed to enhance the sampling of slow collective motions. Compared with PIMD based on thermodynamic integration, this approach removes the need for quadrature and timestep convergence checks, greatly reducing manual effort in the analysis. Applications to malonaldehyde and the HCl dimer yield the most precise reported splittings while reducing the computational cost by several-fold and by roughly three orders of magnitude, respectively. Application to the water dimer provides the first numerically exact path-integral calculations for the ground-state splittings on three different PESs, all obtained simultaneously from a single set of trajectories by reweighting.

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Decoding Water Through Quantum Simulations and Vibrational Spectra

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Water exhibits remarkable structural, thermodynamic, and spectroscopic properties that arise from its complex hydrogen-bond network and many-body molecular interactions. In this talk, I will present our recent efforts toward decoding water from its underlying molecular interactions to its vibrational spectra. I will first discuss the development of high-accuracy many-body potentials for water, highlighting our recent q-AQUA and q-AQUA-pol models. I will then introduce MB-PIPNet, a monomeric machine-learning framework that combines the physical rigor of the many-body expansion, the efficiency of permutationally invariant polynomials, and the scalability of neural networks to enable accurate and efficient molecular simulations. The second part of the talk will focus on quantum vibrational spectra. I will present our work on the vibrational self-consistent field and vibrational configuration interaction (VSCF/VCI) method and its applications to protonated water clusters, and liquid water. In particular, I will show recent VSCF/VCI simulations of liquid-water spectra with local-monomer approaches, providing quantitative interpretations of the fundamental, overtone, and combination bands. The effects of vibrational mode couplings on liquid water structures will also be discussed.

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Semiclassical Vibronic Spectroscopy with New Initial Value Representation Techniques

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We developed a semiclassical initial value representation (SCIVR) method for nonadiabatic real-time dynamics, with a complete derivation starting from coherent-state path integrals. We call it the squeezing SCIVR (sq-SCIVR) because of the new squeezing technique introduced. The method is more norm-conserving, more accurate and more numerically efficient than the previously tested Meyer–Miller–Stock–Thoss Herman–Kluk (MMST HK) method [1]. We applied it to one- and multi-dimensional non-adiabatic models for vibronic spectroscopy, and the results are very encouraging. Our method is able to reproduce the spectra with satisfying accuracy while requiring very little manual adjustment or filtering. Therefore, it shows strong potential for applications to a broader range of non-adiabatic systems.

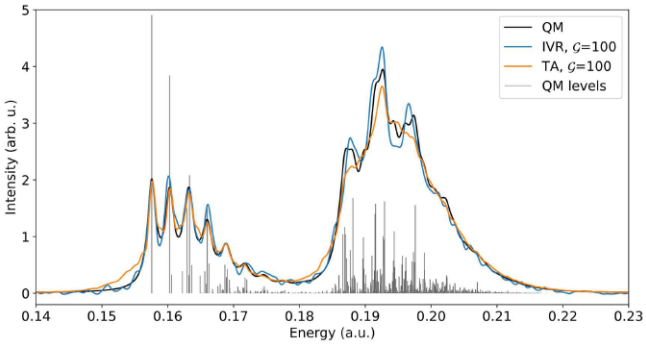

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Figure. The vibronic spectra of the 4-mode pyrazine model calculated with sq-SCIVR, its time-averaging version, and the quantum benchmark.

Stochastic Schrödinger Equation for Carrier Dynamics in Organic Semiconductors

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It is well-known that charge/energy transfer dynamics with strong electron-phonon interactions in organic materials is commonly described by rate theories while that with strong electronic couplings in inorganic semiconductors is dealt with by band theories. However, in novel organic and oxide crystals, electron-phonon and electronic couplings have a similar order of magnitude, and neither rate methods nor band theories are applicable. In this work, I show a rigorous stochastic Schrödinger equation and its approximations proposed by us to bridge the gap between rate and band theories, in which the molecular vibration is introduced as a random fluctuation of the electron energy level, and thus the approach is suitable to the dynamic process in nanoscale systems.[1] We also try to extend the stochastic Schrödinger equation into both the lattice momentum space and the coordinate space, and provide an innovation for carrier dynamics simulations in the field of inorganic semiconductors.[2] Finally, we demonstrate the applications with charge separation in donor-acceptor organic solar cells.[3]

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ABSTRACT

Invited Speakers

PIMD Simulations of Bulk Water and Methane Hydrate with Highly Accurate Neural Network Potentials

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Path integral molecular dynamics can yield quantitatively accurate thermodynamic properties of bulk systems when the underlying potential is sufficiently accurate. In this talk, I will present PIMD results for bulk water and methane hydrate using two highly accurate potentials, both constructed by fitting many-body interaction energies from high-level electronic structure calculations with fundamental-invariant neural networks. The results show unprecedented agreement with experiment.

Unconventional Superconductivity from Lattice Quantum Disorder

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Unconventional superconductivity presents a defining challenge in physics. Prevailing theoretical frameworks have predominantly emphasized electrons, largely neglecting the rich physics inherent in the lattice. Conventional phonon theory omits quantum many-body effects of the nuclei, leading to misleading structural phase diagrams and an unsound foundation for superconducting theory. Here, by incorporating nuclear quantum many-body effects within first-principles calculations, we discover a lattice quantum disordered (LQD) phase in superconductors H_3S and $La_3Ni_2O_7$. This phase occupies a triangular region in the *P-T* phase diagram, whose left boundary aligns precisely with T_c of the left flank of the superconducting dome. Its T_c^{max} coincides with the dome's peak, identifying this phase as both the origin of superconducting transition on the left flank and a key ingredient of the pairing mechanism. Our findings advance the understanding of unconventional superconductivity and establish LQD as a unifying framework, both for predicting new superconductors and for elucidating phenomena in a broader context of condensed matter physics.

We employed the PIMD method to rigorously incorporate nuclear quantum many-body effects. Using the centroid mean force, we obtained the dispersion relation of lattice motion in the LQD region, thereby determining the phase boundary. In a previous work [2], we first proposed this method and verified its accuracy. In the present work [1], we extend the study of the LQD phase to finite temperatures and uncover the decisive influence of LQD on unconventional superconductivity.

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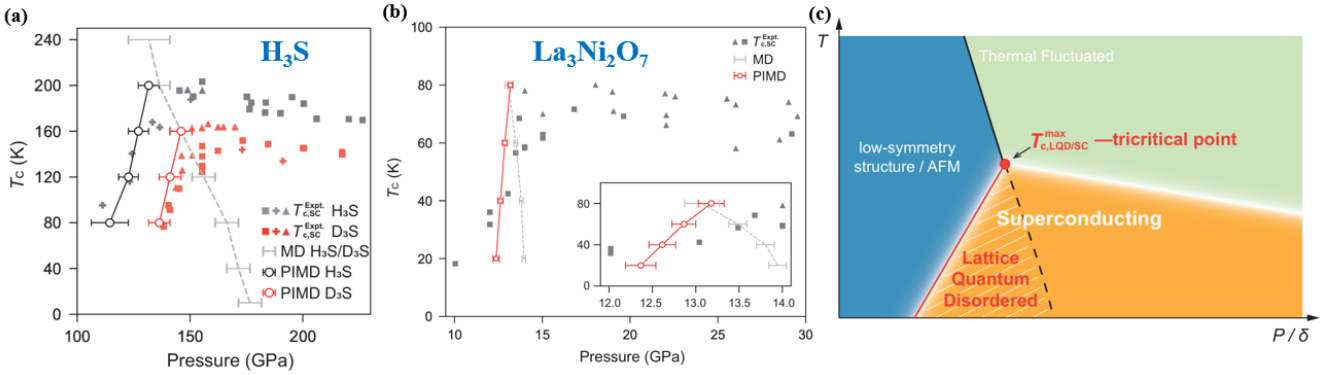

Atomistic Nonadiabatic Reaction Rates from Mean-Field Path Integrals

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Nonadiabatic condensed phase reactions are central to a wide range of interesting chemical processes, such as electron transfer and proton transfer reactions. Although many nonadiabatic dynamic methods have been developed to characterize the reaction rates and mechanisms, accurate atomistic simulations that incorporate the nuclear quantum effects and vibronic couplings remain challenging.

Mean-field ring polymer molecular dynamics (MF-RPMD) provides an effective way to calculate nonadiabatic reaction rates for a real system by propagating the nuclei on an effective electronic state-averaged potential energy surface. However, previous work shows that rates calculated from the MF-RPMD Hamiltonian significantly overestimate the rates in the nonadiabatic regime1. For this presentation, I present our work on a new way of doing mean-field path integral rate calculation for nonadiabatic reactions2. By correcting the reactive flux with respect to the kink configurations, this method yields quantitatively accurate rates for models over a wide range of driving forces and electronic coupling strengths.

Beyond model-system application, I extended MF-RPMD to atomistic condensed phase electron transfer through an implementation with i-PI. I applied this method to an electron transfer between two iron ions in water and compared the resulting rates with Marcus theory across different driving forces. Preliminary results show promising order of magnitude agreement with Marcus theory, with rates that are systematically higher than classical Marcus Predictions due to nuclear tunneling effects. Overall, these results suggest that MF-RPMD provides an efficient and promising framework for simulating atomistic nonadiabatic reactions.

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Electronic Path-Integral Normal Modes of Mapping Representations for Nonadiabatic Dynamics

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Accurate simulation of nonadiabatic dynamics is desirable for understanding ultrafast light and energy transfer. The major challenge for classical scaling mapping methods is simultaneously achieving conservation of the Quantum Boltzmann Distribution (QBD) and Rabi oscillations. For a single surface, Matsubara dynamics truncates in the higher path-integral normal modes of the nuclear variables, resulting in classical, QBD conserving dynamics.1 Nonadiabatic Matsubara dynamics has been proposed,2,3 truncating only in the nuclear normal modes and leaving electronic variables unchanged in the Meyer-Miller-Stock-Thoss (MMST) or spin-mapping representations, which surprisingly do not generally conserve the QBD. Here, we will discuss the first electronic normal mode investigations using the MMST and spin-mapping representations. By focusing on a two-level electronic-only system, we find that truncating in MMST normal modes results in a loss of QBD conservation for a single trajectory and poor dynamics, suggesting that the MMST representation is not optimal for QBD conserving nonadiabatic dynamics.4 However, by utilizing the spin-mapping representation,5 we find the higher normal modes of the spin-vector z-component (the difference in state populations) are constrained by the Boltzmann distribution. We derive the population occupancy correlation function and find the time-evolved observable to be a function of only the spin-mapping centroid, which is propagated in an accurate and symplectic manner.6 Computationally, the full N bead results are replicated using only the spin-mapping centroid, leading to accurate, QBD conserving dynamics. To our knowledge, this is the first QBD conserving method that truncates in electronic normal modes. These developments will aid the future derivation of highly accurate and Quantum Boltzmann conserving nonadiabatic dynamics methods.

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ABSTRACT

Contributed Speakers

Quantum annealing for materials

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Finding the global minimum of a potential-energy surface is a fundamental challenge in materials science, underpinning problems that range from protein folding to the structure of atomic clusters. Quantum annealing (QA) has emerged as a promising global-optimization strategy [1,2], using quantum fluctuations rather than the thermal fluctuations that drive classical simulated annealing. A direct implementation of QA for realistic, multidimensional systems, however, remains computationally demanding because sampling the quantum nuclear density is challenging.

To address this bottleneck, we propose a QA implementation based on path-integral molecular dynamics [3]. The approach retains the flexibility and simplicity of molecular-dynamics simulations while providing an efficient route to explore complex potential-energy landscapes. On benchmark systems, including LennardJones clusters, the method often outperforms its classical counterpart. When combined with machine-learning potentials, it also enables applications to relevant materials-science problems, such as crystal-structure reconstruction.

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A New Path Integral Transition State Theory

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I will present a new path integral transition state theory. This is based on a new rigorous derivation of instanton rate theory from first principles using Matsubara Dynamics which elucidates key physical features of the theory.

The formulation introduces a new class of path-integral dividing surfaces which naturally select the real-time flux along the instanton pathway. A central advantage of the approach is that it captures anharmonic fluctuations around the instanton path non-perturbatively, going beyond the harmonic treatment underlying standard instanton theory.

One-dimensional benchmark calculations show excellent agreement with exact quantum-mechanical calculations for both symmetric and asymmetric systems and the new method outperforms existing methods like quantum and semiclassical instanton theory or RPMD-TST.

In multidimensional systems, it accurately describes ro-vibrational coupling as well as coupling between rotation and permutational degrees of freedom of a path. This allows to describe reactions which have very floppy modes. Likewise, this method enables the computation of exact quantum partition functions. This will be demonstrated with applications to real molecular reactions.

Non-adiabatic Molecular Simulations with Path Integral Monte Carlo

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Non-adiabatic effects play a central role in many chemical processes, including photochemistry, charge transfer, and radiationless relaxation near conical intersections. Here, we present our recently proposed path integral Monte Carlo (PIMC) approach for molecular systems with multiple coupled electronic states [1], where non-adiabatic effects are treated in a diabatic representation. The method accurately reproduces exact results for non-adiabatic model systems and thermodynamic equilibrium properties of simple molecules.

To enable applications to higher-dimensional systems, we additionally discuss ongoing work on machine-learning-based diabatization using neural ordinary differential equations. In this framework, smooth quasi-diabatic potential energy surfaces are constructed through the parallel transport of electronic states, providing a differentiable and geometrically motivated approach for treating non-adiabatic couplings and generating diabatic representations suitable for PIMC simulations.

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Divergence of Semiclassical Expansions: Restoring Spatial Coherence in Density Functional Theory

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This work analyzes the intrinsic errors in standard density functional approximations (DFAs) from the perspective of semiclassical asymptotic analysis. By mapping the density gradient expansion onto the WKB approximation, we show that the nonperturbative tunneling information that can be extracted via Borel resummation[1], indicates an exponential decay of the one-particle reduced density matrix (1-RDM) offdiagonal elements in stretched diatomic molecules. Furthermore, we reveal that standard DFAs fail to capture this nonlocal spatial coherence, thereby yielding a spurious constant error in the non-additive exchange-correlation energy in the dissociation limit. Finally, we show that fragment density functional approximations within partition-DFT[2], such as the overlap approximation[3], successfully reintroduce spatial coherence into approximate DFT, serving as an effective remedy for the fractional-spin and fractional-charge errors in (semi)local DFAs.

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ABSTRACT

Contributed Speakers

Nuclear Quantum Effects as a Denoising Problem

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The imaginary-time path integral rigorously captures nuclear quantum effects (NQEs) through the isomorphism between quantum statistics and a classical ring-polymer distribution. The Euclidean action of the ring polymer separates into a quadratic action which encodes particle mass, chain boundary conditions, and even non-local dissipative bath coupling, and a residual factor determined only by the potential energy surface (PES). Since the quadratic component is known analytically, it can be composed at sampling time with a learned denoiser trained on the PES-defined residual — a classical Boltzmann factor at the single-bead inverse temperature τ. Sampling the path integral therefore reduces to a denoising problem on the classical distribution, and we call this framework the Denoising Path Integral (DPI).

This decomposition implies that the physical conditions governing NQEs can be modified at sampling time without retraining the denoiser. The denoiser operates on each imaginary-time bead at fixed width τ, and adjusting the number of beads P changes the physical inverse temperature according to $\beta = P\tau$. Replacing the quadratic component by changing the particle mass in the quadratic action or by adding a Caldeira–Leggett bath kernel transfers the same denoiser to different isotopes and dissipative environments. As in Ref. [1], the denoiser can be trained from standard molecular dynamics at the single-bead inverse temperature τ or from restrained sampling, bypassing the need to first run path-integral simulations.

We demonstrate DPI on three systems: (i) a dissipative double-well potential coupled to a Caldeira–Leggett bath, where a single denoiser transfers across bath coupling strengths and inverse temperatures, matching reference centroid distributions and radius of gyration; (ii) the Zundel cation ($H_5O_2^+$), where the relative preference of D and T for the central shared site versus terminal sites is predicted over 150–480 K; and (iii) bulk water with 216 molecules, where isotope effects in H_2O, D_2O and T_2O radial distribution functions are predicted within 1% of the reference peak heights.

These results show that NQEs arise naturally by analytically composing the quadratic path structure with a denoiser trained only on standard molecular dynamics data.

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Imaginary Time Path Integral for Fictitious Identical Particles

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Imaginary time path integral is a powerful tool to study the thermodynamics of quantum many body systems. Consequently, researchers have developed path integral Monte Carlo (PIMC) and path integral molecular dynamics (PIMD) to perform *ab initio* simulations of large-scale quantum systems. On the other hand, quantum exchange effects are also important and must be taken into account in PIMC/PIMD for identical particles. Hirshberg et al. [1] have developed a recurrence relation to consider exchange effects in PIMD. However, the notorious fermion sign problem emerges when PIMC/PIMD is applied to Fermi systems. Fictitious identical particle (FIP) [2,3,4,5] became a popular method to circumvent fermion sign problem through extrapolation from the bosonic sector to the fermionic sector, and in this talk I focus on PIMC/PIMD technique for FIP, as well as the applications to different Fermi systems.

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The Quantum Nature of Non-equilibrium Proton Transfer — A Full-wavefunction Dynamics Study

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Non-equilibrium proton transfer is ubiquitous as key step in applied chemistry and biological system. The study of proton transfer mechanism provides general insights into electron-nucleus interplay in condensed phase science. Because of lack of concrete, proper description of the nuclear quantum dynamics, both experiment and theory face challenge in understanding data as well as simulating dynamics. Here, using effective Hamiltonian of full-wavefunction description of proton and electron, and treating effect of surrounding environment by open quantum system, we show in several organic chromophores and water molecule network the dominate role of electron-proton(s) quantum correlation that obeys a vibrionic coupling form. The theory gains quantitative consistency with ultrafast time-resolved spectroscopy, and explains a series of anomalous isotope effects beyond classical/semiclassical theory, showing the nature of proton transfer as coherent evolution among entangled electronproton states. The electron-proton(s) quantum correlation can cause novel proton transport properties, including significant reduction of OH vibrational frequency, nonlocal quantum superposition of two degenerate reactions, and an increasing transport rate with heavier hydrogen mass. These study reveals the discovered electronproton(s) quantum correlation is potentially crucial in proton transfer and general condensed phase chemistry and physics process.

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Herman–Kluk–like Semi-classical Initial-value Representation for Boltzmann Operator

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The coherent-state initial-value representation (IVR) for the semi-classical real-time propagator of a quantum system, developed by Herman and Kluk (HK), is widely used in computational studies of chemical dynamics. On the other hand, the Boltzmann operator $\exp(-\hat{H}/k_BT)$, with $\hat{H}$, k_B, and T representing the Hamiltonian, Boltzmann constant, and temperature, respectively, plays a crucial role in chemical physics and other branches of quantum physics. One might naturally assume that a semi-classical IVR for the matrix element of this operator in the coordinate representation (i.e., $\langle\tilde{x}|\exp(-\hat{H}/k_BT)|x\rangle$, or the imaginary-time propagator) could be derived via a straightforward "real-time → imaginary-time transformation" from the HK IVR of the real-time propagator. However, this is not the case, as such a transformation results in a divergence in the high-temperature limit ($T \to \infty$). In this work, we solve this problem and develop a reasonable HK-like semi-classical IVR for $\langle\tilde{x}|\exp(-\hat{H}/k_BT)|x\rangle$, specifically for systems where either the gradient of the potential energy (i.e., the force intensity) has a finite upper bound or the potential becomes harmonic in the long-range limit. The integrand in this IVR is a real Gaussian function of the positions x and x, which facilitates its application to realistic problems. Our HK-like IVR is exact for free particles and harmonic oscillators, and its effectiveness for other systems is demonstrated through numerical examples.

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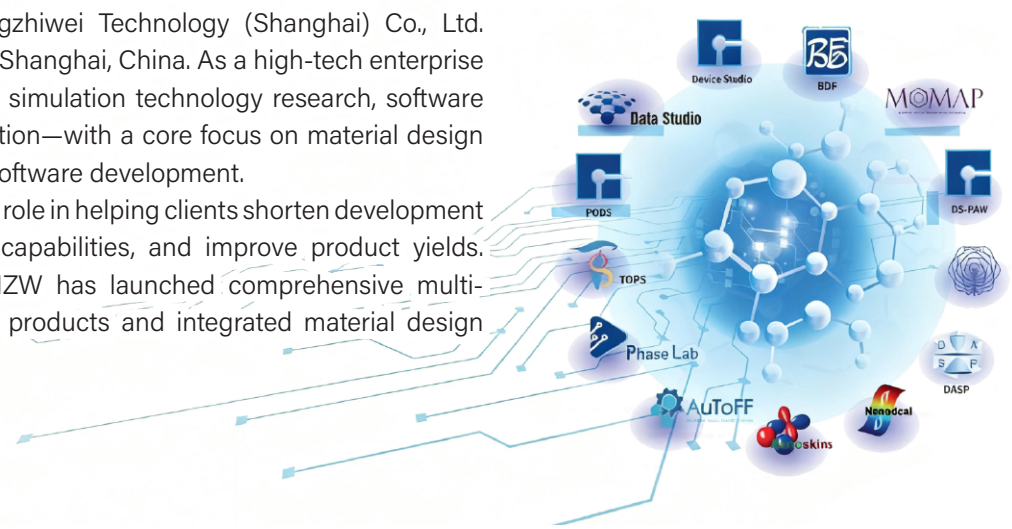

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