UCMERCED | CHEMISTRY & BIOCHEMISTRY

DATE 02/06/2026 | TIME 01:30pm | LOCATION SSB 170

CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES

Quantum Dynamics with Gaussian Bases: Theme and Variations

Abstract:

Importance of the quantum-mechanical effects associated with the nuclei is gaining recognition in chemistry and physics, as researchers manipulate matter, light, electric and magnetic fields at the atomistic level for advanced materials applications. For example, the isotope dependence of the proton conductance in low-dimensional boron nitrides, and of the crystallinity of poly(3-hexylthiophene) is attributed, in part, to the nuclear quantum effects. The development of a general dynamics approach, incorporating the nuclear quantum effects and scalable to large molecular systems, remains an outstanding theoretical challenge because of the exponential scaling of computational costs with the system size. We will discuss application or the time-dependent variational principle to the trajectory-driven bases, and describe exact and approximate dynamics, inspired by the quantum trajectory formulation of the Schrödinger equation [1,2]. The significance of the quantum behavior of the nuclei will be illustrated on the case study of the Kinetic Isotope Effect in Cytochrome P450 Decarboxylase OleT [3], attributed in part to quantum tunneling.

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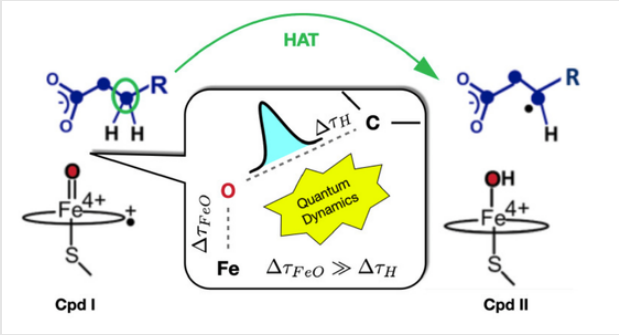
References

[1] M. Dutra, S. Wickramasinghe, and S. Garashchuk. Quantum Dynamics with the Quantum Trajectory-Guided Adaptable Gaussian Bases. Journal of Chemical Theory and Computation 16, 18-34 (2020). DOI: 10.1021/acs.jctc.9b00844

[2] S. Garashchuk, J. Stetzler, C. Jayawardana, M. Safo, V. Rassolov. Variational Dynamics of Multicomponent Wave Functions Represented in a Basis Driven by a Time-Dependent Gaussian Wavepacket. J. Chem. Theory Comput. 21 (15), 7249-7266 (2025) DOI: 10.1021/acs.jctc.5c00640

[3] M. Dutra, et al. Experimental and Theoretical Examination of the Kinetic Isotope Effect in Cytochrome P450 Decarboxylase OleT. J. Phys. Chem. B 126 (19), 3493-3504 (2022). DOI: 10.1021/acs.jpcb.1c10280.



About the Speaker:

M.S., 1992, Moscow Institute of Physics and Technology, RF
Ph.D., 1999, University of Notre Dame, IN, USA
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Visiting Scientist at Max Planck Institute for Physics of Complex Systems, Germany (2023), California Institute of Technology (2016), University of New South Wales-Canberra, Australia (2016); USC Rising Star, 2012; Doctoral New Investigator ACS Petroleum Research Fund 2011; National Science Foundation Career, 2011.

Research Interests:

Theoretical and computational chemistry focusing on quantum effects in dynamics of nuclei, development of approximate quantum trajectory dynamics method scalable to large molecular systems, incorporation of the zero-point energy, quantum tunneling, and other quantum effects in reactive dynamics.

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