Physical Chemistry Seminar

Bridging Quantum and Classical: An Efficient Framework for Capturing Zero-Point Effects in Hydrogen-Related Chemistry

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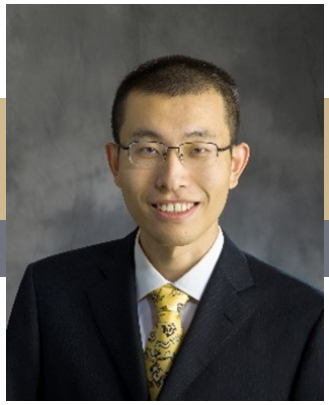

Zero-point effects — quantum mechanical phenomena arising from the fact that nuclei never truly stand still, even at absolute zero — are essential for accurately describing many chemical and biological processes, especially those involving hydrogen. Yet, capturing these effects in large-scale molecular simulations remains a major challenge. To address this, we developed the Constrained Nuclear-Electronic Orbital (CNEO) framework, which incorporates zero-point effects along with certain other components of nuclear quantum effects directly into quantum chemistry calculations and molecular dynamics simulations, while maintaining computational efficiency.

Our methods — CNEO density functional theory (CNEO-DFT) and CNEO molecular dynamics (CNEO-MD) — significantly outperform conventional DFT and ab initio MD in predicting vibrational spectra, particularly for hydrogen-dominated modes. With CNEO transition state theory (CNEO-TST), we achieve more accurate hydrogen/proton/hydride transfer rate predictions at little additional cost. CNEO simulations with periodic boundary conditions also reveal shifts in hydrogen adsorption preferences on metal surfaces driven by zero-point effects. We have also extended the framework to excited-state calculations, nonadiabatic dynamics, and hybrid QM/MM calculations. Together, these developments establish CNEO as a versatile and efficient tool for bridging classical simulations with a quantum mechanical description of nuclear motion.

Wednesday, October 1, 2025 **10:30am** **BRWN 4102**

PURDUE UNIVERSITY | James Tarpo Jr. and Margaret Tarpo Department of Chemistry

Yang Bio

Yang Yang is an Assistant Professor of Chemistry at the University of Wisconsin-Madison. He holds dual bachelor's degrees in chemistry and physics from Peking University (2011) and earned his Ph.D. in theoretical chemistry under the mentorship of Dr. Weitao Yang at Duke University (2016). Following his doctoral work, he pursued postdoctoral research with Dr. Sharon Hammes-Schiffer at the University of Illinois Urbana-Champaign and Yale University before joining the UW-Madison faculty in 2019.

Dr. Yang's research focuses on advancing multicomponent quantum theories to describe systems with significant nuclear quantum effects, particularly zero-point effects. His group has pioneered the Constrained Nuclear-Electronic Orbital (CNEO) framework, enabling the accurate and efficient incorporation of nuclear quantum effects in quantum chemistry calculations and molecular dynamics simulations. In recognition of his innovative contributions, Dr. Yang received the NSF CAREER Award in 2022.