UCMERCED | CHEMISTRY & BIOCHEMISTRY

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CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES:

Including Nuclear Quantum Effects in Condensed Phase Systems via Path-Integral Methods

Abstract:

Nuclear quantum effects such as tunneling and nuclear zero-point energy are important components in obtaining accurate structural and dynamic properties for a host of chemical processes including charge and energy transfer reactions, the behavior of molecules under confinement, and systems with hydrogen bonding networks. However, most traditional computational methods, like ab-initio molecular dynamics, do not include quantum effects in the nuclear degrees of freedom. Path-integral based methods, like path-integral molecular dynamics, are a class of methods that capture nuclear quantum effects through replacing a quantum particle with an n-bead classical ring polymer. Here, I present our work on expanding path-integral methods into a new atomistic path integral molecular dynamics software program where each atom in a system can be treated with a different quantization level. This method can drastically improve the computational scalability of path integral methods and allows for the simulation of previously inaccessible condensed phase systems. I will also discuss our work on expanding path integral methods into multi-electronic state systems through a mean-field approach. This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division, Condensed Phase and Interfacial Molecular Science program, FWP 16249.

Britta Johnson

Computational Scientist, Physical Sciences Division

Pacific Northwest National Laboratory (PNNL)

About the Speaker:

Britta A. Johnson earned her B.A. in Chemical and Mathematical Physics under the direction of Prof. Robert J. Hinde at the University of Tennessee in 2012. She received her Ph.D. in Chemistry with Prof. Edwin L. Sibert III at the University of Wisconsin, Madison in 2017. From 2018 to 2021, Britta completed a postdoctoral fellowship with Prof. Nandini Ananth at Cornell University. She joined the staff at the Pacific Northwest National Laboratory as a computational scientist in the Physical Sciences Division in 2021. Britta's research focuses on the development and implementation of methods to treat nuclear quantum effects in condensed phase systems. In particular, she is focused on using path-integral based methods to simulate charge and energy transfer reactions and interfacial systems.

For more info, contact: Liang Shi, lshi4@ucmerced.edu