Designing Quantum Chemistry Methods with and Beyond Chemical Intuition

Seminar

Friday,
November 22, 2024

2:00 – 3:00 p.m.

Beaupre Center,
Room 105

Quantum chemistry simulations are essential for connecting electron-level behaviors to macroscopic chemical phenomena, such as chemical reactions, spectroscopy, and electromagnetic properties. However, balancing computational cost and accuracy remains challenging, especially for strongly correlated electrons. In this talk, I will discuss how the complexity of the electronic structure impedes universal, scalable solutions and propose guidelines for designing efficient quantum chemistry methods using chemical intuition. I will illustrate these guidelines through two methods I developed. First, I will introduce density matrix embedding theory (DMET) and its finite-temperature extension, demonstrating how understanding the entanglement structure helps reduce computational costs. Second, I will present a new multi-reference approach that connects strong and weak electron correlations via a non-orthogonal configuration interaction (NOCI) formulation, showing how capturing different types of electron correlations enhances accuracy. Moving beyond chemical intuition, I will then explore the potential for a universal quantum chemistry method. Our recent development of a neural network quantum state (NNQS) with a generative model based on normalizing flows illuminates the path toward universal solutions in quantum chemistry. Finally, I will share my perspective on the evolving role of quantum chemistry: from making accurate predictions to enabling active chemical discovery.

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Fall 2024 Seminar Series

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