Unconventional descriptions of correlated electrons with balanced accuracy and efficiency

Seminar

Monday, November 25, 2024

3:00 – 4:00 p.m.

Beaupre Center, Room 105

Electron correlation, the quantum many-body nature of electrons not captured by the mean-field approximation, remains the central challenge in modern quantum chemistry. Its accurate and efficient description holds the promise of accelerating discoveries in transition-metal and f-block chemistry, where electron correlation effects are especially prominent. In this talk, I will present my work on addressing this challenge by developing unconventional methods and algorithms motivated by physical insights and mathematical rigor. First, I will demonstrate the importance of screening effects for capturing dynamic correlation. I will showcase the success of the random phase approximation and its screened exchange correction in describing noncovalent interactions and guiding catalyst design. Second, I will show how symmetry projection can account for static correlation. I will highlight a reformulation of Wick's theorem that ensures efficient and numerically robust implementations of symmetry-projected methods. Finally, I will discuss bridging the treatments of these two aspects of electron correlation to develop theories with balanced accuracy and efficiency.

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Fall 2024 Seminar Series

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