

Exploring Quantum Chemistry Across Representations

Seminar

Monday

Nov. 16, 2026

3:00 – 4:00pm

Beaupre Center,

Room 105



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I will discuss a concept I call operator alchemy (OA), which helps us understand quantum chemical systems by exploring them beyond their native representation to reveal simpler structures or more efficient simulation pathways. The resulting quantum transformations can help untangle the complexity of various chemical problems, initiate cross-pollination between different scientific areas, and enable implementation on various quantum devices. I will demonstrate the potential of OA in three parts with transformations involving fermions (e.g., electrons), bosons (e.g., molecular vibrations), and qubits (e.g., nuclear spins).

In the first part, I will discuss how electron pairing is important for understanding strong electron correlation, a scenario in which electron interactions are far from the simple molecular orbital picture, which is important in understanding various phenomena ranging from nitrogen fixation to superconductivity. Then I will show that electron pairs can be naturally mapped to qubits, initiating interactions between developments in fermion pairing and quantum information science. In the second part, I will focus on fermion-to-boson transformations to enable molecular electronic calculations on bosonic quantum devices, which is a rapidly progressing field of quantum computing architecture. Finally, I will discuss how time evolution of qubit systems, related to computational simulations of NMR experiments among other applications, can be implemented more efficiently when they are mapped to a fermionic representation. Together, these transformations will illustrate how OA can reveal new computational strategies for diverse chemical problems.