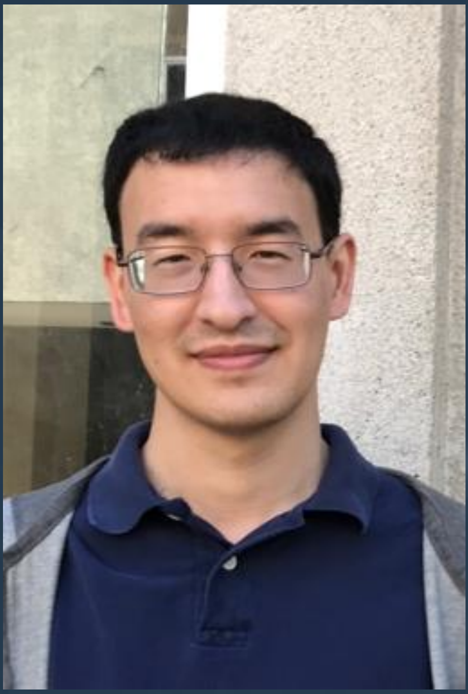
RICE QUANTUM GROUP MEETING SEMINAR SERIES

Targeting Excited States with Auxiliary Field Quantum Monte Carlo



May 30th, 2025, 12 – 1:30 PM
SST 300

Leon Otis

Prof. James Shee group

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Leon Otis is a postdoctoral researcher in the group of Professor James Shee. He obtained his Ph.D. from the University of California Berkeley working in the group of Professor Eric Neuscamman. His research focuses on the development and application of electronic structure theory methods for excited states in both molecular and solid-state systems, with a particular interest in quantum Monte Carlo and quantum embedding techniques.

ABSTRACT

Electronic excited states play a key role in a wide variety of phenomena and applications including nanoscale catalysis, photovoltaics, and solid-state qubits. However, theoretical tools for describing excited states remain less fully developed compared to those for the ground state and obtaining accurate excitation energies across different types of excited states is often challenging for the most commonly used electronic structure methods. I will present work exploring auxiliary field quantum Monte Carlo (AFQMC) as a promising approach for excited states with initial tests on a set of doubly excited states in small molecules. I will also discuss the role of the trial wave function used in AFQMC as well as methodological improvements using correlated sampling and variance matching.

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