RICE QUANTUM GROUP MEETING SEMINAR SERIES

Designing Computational Methods for Strongly Correlated Electrons

Chong Sun

Prof. Gustavo Scuseria group
Department of Chemistry

Dr. Chong Sun is a postdoctoral fellow with Professor Gustavo Scuseria in the Department of Chemistry at Rice University and holds a joint position as a research assistant at Microsoft Quantum. Her research focuses on advancing chemical and physical simulations through quantum chemistry, artificial intelligence (AI), and quantum computing. Dr. Sun earned her Ph.D. from the California Institute of Technology under the supervision of Professor Garnet Kin-Lic Chan, where she developed computational frameworks for strongly correlated electrons. Currently, she is integrating electronic structure theory and generative models to discover novel quantum materials, emphasizing noise-resilient materials for quantum computing.

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ABSTRACT

Computational simulations are now essential for studying molecules and quantum materials. However, balancing computational cost and accuracy remains challenging, particularly in scalable simulations for strongly correlated systems. In this talk, I will discuss guidelines for designing efficient methods tailored to these systems from a quantum chemist's perspective. I will illustrate these guidelines through two methods I developed, FT-DMET (finite-temperature density matrix embedding theory) and SNOCISD (selected non-orthogonal configuration interaction with single and double excitations). Through this talk, my goal is to convey the current landscape of electronic structure theory and explore connections between our methods and potential applications within the RQI groups.