Physical Chemistry Seminar

Wenjie Dou

Assistant Professor of Chemistry and Physics | Westlake University in China

Excited-state Electronic Structure and Non-adiabatic Dynamics for Molecular Spin Systems

The electronic structure theory and non-adiabatic dynamics of complex systems are very challenging due to the steep scaling of the current computational methods. In the first part of the talk, I will present our newly developed stochastic second-order coupled cluster method (sRI-CC2) for calculating the excited state of large systems. Using the set of stochastic orbitals, we decouple the crucial 4-index electron repulsion integrals into stochastic resolution of identity. These techniques allow a remarkable scaling reduction from O(N^5) to O(N^3), which allows us to calculate the excited state properties for systems with thousands of electrons. In the second part of the talk, I will present a dynamical approach for open quantum systems—Memory kernel coupling theory. This approach builds upon the memory kernel formalism and avoid the calculation of projected dynamics by further decomposing the memory kernel into auxiliary kernel functions. We employ this approach to study the spin-phonon relaxation process in a molecular qubit. The numerical results successfully explain novel spin relaxation phenomena observed in experiments.

PHYSICAL SEMINAR

Wenjie Dou's Biography

Wenjie Dou earned a B.S. in physics from the University of Science and Technology of China in 2013 and a Ph.D. in theoretical chemistry from the University of Pennsylvania in 2018. His Ph.D. work focused on modeling non-adiabatic dynamics near surfaces. From 2018 to 2020, he was a postdoc at UC Berkeley working on stochastic implementation of electronic structure theory. He started his independent career at Westlake in Jan. 2021. He is the recipient of 2026 ACS OpenEye/Cadence Outstanding Junior Faculty Award as well as 2025 Tang Ao-Chin Youth Award in Theoretical Chemistry from Chinese Chemical Society. His research interests are non-adiabatic dynamics, excited-state electronic structure, and open quantum systems.