Molecular Electronic Structure at the Nexus of Classical and Quantum Computing

Francesco A. Evangelista, Renke Huang, Jonathon P. Misiewicz, Ilias Magoulas

Department of Chemistry and Cherry Emerson Center for Scientific Computation
Emory University, Atlanta, Georgia, USA

Despite considerable advancements in quantum chemistry, modeling highly entangled molecular states, such as those encountered in bond-breaking processes, excited electronic states, and open-shell species, remains a formidable computational challenge. Quantum computers present a promising solution to this problem, as they can efficiently represent and manipulate entangled quantum states. In this talk, I will highlight hybrid quantum-classical approaches for molecular electronic structure developed by our research group. Specifically, I will introduce the Projective Quantum Eigensolver (PQE), a novel quantum algorithm for trial-state optimization on near-term noisy quantum computers competitive with variational quantum algorithms. Additionally, I will discuss unitary downfolding approaches that maximize the potential of existing quantum hardware for accurate quantum computations, showcasing the remarkable reduction of quantum resources in the case of a simple organic chemistry reaction. These new techniques, in combination with more accurate hardware and a larger number of qubits, will provide a systematic path to predictive simulations of chemical reactivity.