Physical Chemistry Seminar

Adaptive Variational Ansatz to Study Open Quantum Systems Dynamics

Saurabh Shivpuje

Graduate Student
Kais Group
Purdue University

The rapid advancement of quantum computing has opened transformative possibilities for simulating material and chemical systems. A key frontier in this field is the study of open quantum systems, which account for environmental interactions leading to non-unitary evolution. Conventional quantum computing techniques, designed primarily for unitary processes, struggle to capture these dissipative effects that are essential for realistic modeling of molecular, photonic, and condensed-matter systems. Variational Quantum Algorithms (VQAs) have emerged as a promising approach by leveraging hybrid quantum–classical optimization to model such dynamics efficiently on near-term hardware. Among these, adaptive variational ansatz methods, capable of dynamically constructing expressive quantum circuits, have shown promise in addressing the challenges of open-system evolution.

In this talk, I present the Unrestricted Adaptive Variational Quantum Dynamics (UAVQD) framework, together with a stochastic Schrödinger equation (SSE)-based trajectory approach, to simulate non-unitary quantum dynamics. The adaptive ansatz construction ensures computational efficiency while maintaining accuracy through the McLachlan variational principle, while the trajectory-based method demonstrates how ensemble averages of pure-state simulations can effectively reproduce Lindblad dynamics. Together, these adaptive frameworks provide a versatile and accessible pathway for investigating a wide range of open-system phenomena, paving the way for future applications in quantum chemistry, photonics, and complex quantum materials.

Wednesday, November 19, 2025 **10:30am** **BRWN 4102**

PURDUE UNIVERSITY | James Tarpo Jr. and Margaret Tarpo Department of Chemistry