Quantum-Classical Hybrid Computing to Design Materials

Quantum simulators offer a pathway to applying quantum computational methods to materials science, catalysis, and computational chemistry. In this talk, I will present our efforts to develop versatile quantum simulators capable of addressing complex scientific problems beyond the scope of classical computing. Using quantum optics and neutral atomic systems, we realize high-fidelity simulations of molecules and catalysts. Our approach combines hardware platform design, the development of hybrid quantum-classical algorithms, and systematic validation of simulator performance. The results highlight the potential of our simulators to achieve unprecedented accuracy and efficiency in quantum simulations. Furthermore, we integrate scalable technologies such as integrated optics and hybrid classical-quantum interfaces to enhance simulation capabilities. This presentation will outline our methodologies, interdisciplinary collaborations, and the potential of our quantum simulators to accelerate the discovery of candidate materials for hydrogen energy catalysis.