Predicting and Controlling Scalable Quantum Systems

Abstract:
Quantum matter hosts spectacular excited-state and nonequilibrium effects, but many of these phenomena remain challenging to control and, consequently, technologically underexplored. My group's research, therefore, focuses on how quantum systems behave, particularly away from equilibrium, and how we can harness these effects. By creating predictive theoretical and computational approaches to study dynamics, decoherence and correlations in quantum matter, our work could enable technologies that are inherently more powerful than their classical counterparts ranging from scalable quantum information processing and networks, to ultra-high efficiency optoelectronic and energy conversion systems. In this talk, I will present work from my research group on describing, from first principles, the microscopic dynamics, decoherence and optically-excited collective phenomena in quantum matter at finite temperature to quantitatively link predictions with 3D atomic-scale imaging and quantum spectroscopy. Capturing these dynamics poses unique theoretical and computational challenges. The simultaneous contribution of processes that occur on many time and length-scales have remained elusive for state-of-the-art calculations and model Hamiltonian approaches alike, necessitating the development of new methods in computational physics. I will show selected examples of our approach in ab initio design of active defects in quantum materials, and control of collective phenomena to link these active defects. Finally, I will discuss ideas in directly emulating quantum information systems, particularly addressing the issues of model abstraction and scalability, and present an outlook on various co-design strategies with algorithms efforts underway.

References: