Building the Computational Toolbox for Quantum Materials:
Precise First-Principles Calculations of Electron and Spin Dynamics

Marco Bernardi, California Institute of Technology

Combining density functional theory with many-body techniques is enabling rapid advances in first-principles calculations of electron dynamics in materials. Yet, quantum materials present new challenges because of their intricate structure and electronic interactions.

In this talk, I will present new methods to model electron interactions, transport, and spin dynamics from first principles, emphasizing their relevance to quantum materials. We will focus on: 1) electron-phonon (e-ph) interactions and transport in transition metal oxides with strong electron correlations and/or strong e-ph coupling; 2) precise predictions of electron spin relaxation times from spin-phonon interactions, using a new approach that unifies the description of spin-flip and spin precession mechanisms; 3) leveraging data-driven methods to compress electronic interactions and significantly speed-up their computation.

The talk will conclude with a discussion of PERTURBO, an open source code developed in my group which provides quantitative tools to study electron interactions and dynamics in both conventional and quantum materials.