UCLA College | Physical Sciences Chemistry & Biochemistry

PHYSICAL CHEMISTRY SEMINAR

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University of California, Santa Barbara

Monday, November 21st, 2022
4:00 PM | YH 4222

Bhaumik Collaboratory
Yoo Seminar & Conference Room

Excitation dynamics driving the electronic structure of molecules and solids

Abstract: Capturing the dynamics of electronic excitations in realistic systems containing more than a few electrons is one of the outstanding theoretical challenges. Dynamical quantum correlations mediate interactions and couplings between multiple excited states in materials and represent an important driver of their optoelectronic characteristics. A predictive ab-initio theory is thus critical for understanding, predicting, and designing novel compounds with tailored (quantum) properties. I will discuss how to tackle the first-principles description of excitation dynamics in systems with thousands of electrons and study individual excited states, including their non-trivial interactions. I will exemplify these approaches in practical applications to quantum materials, e.g., exploring the correlated phenomena for localized moire states in twisted bilayer graphene and defect centers in diamond. Our theoretical framework uses real-time methods combined with ab-initio dynamical downfolding. Together with efficient low-scaling numerical techniques, it is generally applicable to (quantum) material science and chemistry problems and constitutes an ideal platform for simulating complex nanoscale systems, such as molecular assemblies or materials interfaces.

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