Title: **Excited-State Phenomena in Organic Materials and at Interfaces from First Principles**

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Abstract:

Organic semiconductors are highly tunable, chemically diverse cheap-to-process materials with promise for next-generation optoelectronics. They also harbor interesting excited-state phenomena such as singlet fission, whereby a singlet exciton decays into two spin-correlated triplets, a mechanism of significant interest for achieving efficiencies beyond the Shockley-Queisser limit of conventional solar cells. Further development of new organic materials requires new intuition that links atomic- and molecular-scale morphology to underlying excited-state properties and phenomena, and integrated studies involving theory and experiments. In this talk, I will discuss two classes of new ab initio methods for calculating excited-state properties of organic crystalline solids and interfaces. First, I will describe the use of a predictive, first-principles Bethe-Salpeter framework for understanding the morphology dependence of multiexciton effects, such as singlet fission, in acene crystals, such as pentacene, tetracene, and TIPS-pentacene. Second, I will cover the use of a new class of tuned hybrid functionals for predicting spectroscopic properties of acene crystals and level alignment at metal-molecule interfaces with density functional theory. Direct connections with experiments will be drawn in all cases.