



Excited States And Energy Conversion In Organic Crystals And At Interfaces Via First-Principles Methods

Prof. Jeffrey Neaton

Department of Physics
University of California, Berkeley

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4:15 – 6:15pm

Pfizer Lecture Hall

Mallinckrodt Building (12 Oxford Street)

Organic crystals and hybrid interfaces are highly tunable, diverse classes of cheap-to-process materials with promise for next-generation optoelectronics. Further development of new materials requires new intuition that links atomic- and molecular-scale morphology to underlying excited-state properties and phenomena. I will review ab initio methods for calculating excited-state and transport properties of crystalline solids and interfaces, and show several applications, where we have used these methods to explain or drive new experiments. Specifically, I will cover the use of first-principles density functional theory with tuned hybrid functionals, and many-body perturbation theory within the GW approximation and the Bethe-Salpeter equation approach, for computing and understanding spectroscopic properties of acene crystals, including new insights into measured multiexciton phenomena such as singlet fission; as time permits, I will additionally share preliminary results on low-dimensional materials, such as 2d chalcogenides, and halide perovskites. I will also discuss multiple approaches to calculating level alignment at metal-molecule interfaces, where we have recently generalized optimally-tuned range-separated hybrid functionals to treat the electronic structure with accuracy comparable to many-body perturbation theory, and describe implications for single-molecule junction transport measurements.