



Monday, March 4, 2019, 12:00 pm
Seaver Science Library, Room 150
SSC Auditorium next to the library

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Electronic Excitations in Materials: From Photovoltaics to Plasmonics

Understanding excited state phenomena is at the heart of many important materials problems, such as photovoltaics, photocatalysis, plasmonics and solid-state lighting. In the realm of modeling and simulations, time-dependent density functional theory (TDDFT) has become one of the most powerful, versatile and popular tools for probing electronic structure and excitations in molecular and solid-state materials. Unfortunately, TDDFT is computationally demanding, and its application to realistic materials remains exceedingly difficult. I will outline our recent progress in developing accurate and efficient TDDFT methods to start addressing these challenges. Among them, we developed a subspace TDDFT method to calculate both excitation energy and excited state forces accurately for systems containing up to a few thousand electrons. We have also developed a time-dependent orbital-free DFT (TD-OFDFT) method with which tens of thousands of electrons can be treated fairly accurately in metals. Combining these TDDFT methods with non-adiabatic molecular dynamics, one can perform coupled electron-ion and exciton-ion dynamics where phonons are important in electron transitions and excitations. I'll show how these first-principles methods can be brought to bear on critical scientific problems that are of broad practical interests, including spontaneous electron-hole separation in perovskite solar cells upon photon adsorption, exciton diffusion and dynamics in disordered semiconductors for organic photovoltaics and plasmonic responses of metallic nanostructures.

Hosted by Professor Oleg Prezhdo

The scientific community is invited

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