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Beyond Density Functional Theory Excited---State Tools for Materials Design

Abstract: First principles computational approaches based on quantum mechanics provide an accurate means for connecting chemical composition, atomic structure, and material properties, allowing for physically motivated design of new materials. The standard first---principles approach for solid---state materials is density functional theory (DFT), which has proven to be rather accurate for describing many material properties. However, standard DFT functionals fail to describe excited---state properties within solids. Alternatively, many---body perturbation theory within the GW and Bethe--- Salpeter Equation (GW/BSE) approach has been shown to predict, with quantitative accuracy, the excited---state properties of many classes of materials. In this talk, I will discuss the accuracy of common numerical approximations within GW/BSE for traditional inorganic semiconductors. Additionally, I will present the application of GW/BSE to organic semiconductors, a class of materials that is especially difficult to describe because of the dominance of weak, long---range electronic interactions. Lastly, I will describe the development of a range---separated hybrid DFT functional with GW accuracy for organic materials.

Bio: Dr. Sahar Sharifzadeh is an Assistant Professor within the Electrical and Computer Engineering and Physics Departments and the Materials Science and Engineering Division of Boston University. She obtained her PhD from Princeton University in 2009 before joining Lawrence Berkeley National Laboratory as a postdoctoral fellow and subsequently project scientist. She joined Boston University in 2014. Her research interests are in understanding and predicting material properties using first---principles electronic structure theories. Her current focus is on characterization and manipulation of the excitonic properties of solid---state materials, using density functional theory and many---body perturbation theory.