Making Organic Electronics Simpler

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This talk outlines our recent theoretical work on (1) the theory of charge transport in polymeric semiconductors and (2) the theory of charge generation in organic photovoltaics. It will describe our attempt to achieve a balanced and useful theory for organic electronics combining highly detailed models with more qualitative theories. The talk will focus on the results that challenge the established views on transport in disordered materials and free charge generation in OPV devices.

The Many-Body Path Towards Quantitative Modeling of Complex Adsorption Systems

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Reliable (accurate and efficient) modeling of the structure, stability, and electronic properties of complex adsorption systems remains a daunting task for modern electronic structure calculations. In the context of approximate density-functional theory, two thorny issues prevent us from reaching the goal of quantitative predictions: the (in)famous self-interaction error and the lack of reliable methods for an accurate description of van der Waals (vdW) interactions for hybrid organic/inorganic systems (HIOS).

Both issues arise from the complexity posed by many-electron quantum mechanics, thereby demanding effective and novel solutions. Focusing on the role of vdW interactions, our recent developments of approximate many-body methods will be discussed along with a few surprises we found when applying these methods to HIOS: (1) The vdW energy can contribute more to the binding of covalently bonded systems than it does for physisorbed molecules; (2) the physically bound precursor state for aromatics on Pt(111) can be more stable than the corresponding chemisorbed state; (3) many-body vdW interactions lead to a binding energy for a fullerene molecule adsorbed on multi-layered graphene that decreases as a function of the number of underlying graphene layers.

Finally, we discuss the challenges that lie ahead on the path towards fully quantitative many-body modeling of complex adsorption systems.