Quantum simulations of organic photovoltaic compounds

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Photovoltaics cells based upon plastic organic semiconducting materials are emerging in the landscape of renewable energies. Although such devices exhibit lower efficiencies than their crystalline-silicon and thin-film counterparts, organic junctions enable the design of inexpensive, light-weight, flexible solar panels. At the nanoscale, photoelectric conversion mechanisms in organic materials differ drastically from photoconversion processes in inorganic semiconductors owing to reduced dielectric screening between photogenerated charges. Gaining physical insight into the complex phenomena involved in separating and collecting photogenerated charges would have significant implications for the development of organic photovoltaic devices (and related nanotechnologies, such as organic light-emitting diodes and organic field-effect transistors). In addition, the fundamental study of photoelectric mechanisms in organics represents an exceptional avenue for electronic-structure methods towards improving and exploring their predictive capacity. In this presentation, I will discuss the essential bottlenecks that had precluded the reliable quantum description of semiconducting organic materials and I will present computational strategies that have been or are currently being developed to address some of these fundamental limitations.

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Preferred: Oral presentation