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Looking for structure/property relations in OPV systems: a multi-level computational approach

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Abstract:

Organic electronics is set to become a major focus of academic and industrial research as it touches a diverse array of important technological fields spanning energy production and storage, computing and consumer electronics. The promise held by organic materials can be delivered if protocols able to speed up materials search are developed. The role of computational material modelling is therefore fundamental. The goal is to predict the relevant properties of a material at the molecular level with the appropriate inclusion of the environment, which may severely affect the performance by suppressing certain mechanisms or by promoting some others not displayed in isolated systems. Only an approach able to include an adequate description of the molecular surroundings allows, in principle, a reliable prediction of most macroscopic properties relevant to the envisioned application. The case of organic photovoltaics (OPV) is emblematic, since it requires an accurate molecular modelling of the electronic structure of the materials (donor and acceptor) at both ground and excited electronic states, as well as the modelling of the effects of short- and long-range interactions on this structure modulated by the morphology of the system.

In this context, we have developed throughout the years, a multi-level computational protocol which allows the prediction and rationalization of a number of key parameters (such as absorption spectra, structural features, hole/e^- transport efficiencies) for photoactive molecules used in OPV set in a variety of environments (solution, donor-acceptor interfaces, thin-films, crystals). The efficacy of the protocol will be illustrated by presenting its applications to a wide range of materials and conditions found in OPV devices, including photoactive polymers [1], small-molecule donors [2,3], molecular dyads for single-material solar cells [4] and non-fullerene acceptor/donor interfaces [65.

References:

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