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Discovering New Organic Materials through Computational Methods

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Abstract : Organic semiconductors have attracted the attention of the scientific community in the past decades due to their unique physicochemical properties, allowing new designs and alternative device fabrication methods. Until today, organic electronic devices are largely based on conjugated polymers mainly due to their easy processability. In the recent years, due to moderate ET and CT efficiencies and the ill-defined nature of polymeric systems the focus has been shifting to small conjugated molecules with well-defined chemical structure, easier control of intermolecular packing, and enhanced CT and ET properties. It has led to the synthesis of new small molecules, followed by the growth of their crystalline structure and ultimately by the device preparation. This workflow is commonly followed without a clear knowledge of the ET and CT properties related mainly to the macroscopic systems, which may lead to financial and time losses, since not all materials will deliver the properties and efficiencies demanded by the current standards. In this work, we present a theoretical workflow designed to predict the key properties of ET of these new materials prior synthesis, thus speeding up the discovery of new promising materials. It is based on quantum mechanical, hybrid, and classical methodologies, starting from a single molecule structure, finishing with the prediction of its packing structure, and prediction of properties of interest such as static and averaged excitonic couplings, and exciton diffusion length.

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