Conceptual Framework of Molecular Electronics

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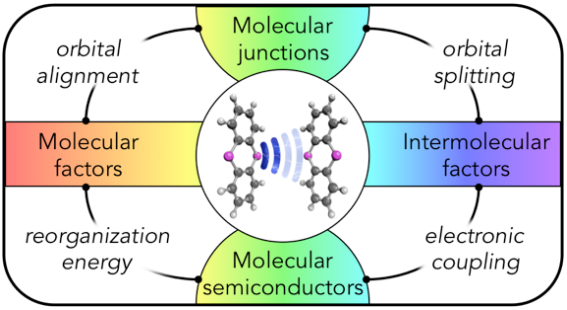
Abstract

Non-covalent interactions are important across a range of organic electronic materials, from molecular semiconductors (e.g., the crystalline organic semiconductors) to molecular junctions (such as dimer bridges in scanning tunnelling microscope experiments). These intermolecular interactions depend on the nature of molecular cores and define not only the stability of their non-covalent assembly, but also its charge transport properties.[1]



In the present contribution, we draw a parallel between the transport in the nanogap between metallic electrodes and charge carrier mobility in the bulk of an organic semiconductor.[2] We show that, within the model approximations, the same systems are consistently among the best and the worst performers, with similar principles guiding their performance in the two types of materials. More generally, we establish a conceptual framework for various non-covalent molecular electronic architectures that connects intrinsic properties of molecular cores with the properties of their non-covalent assemblies (see Figure). These results demonstrate the unifying footprint of the fundamental electronic structure of molecular cores on the diverse charge transport properties and offer the design strategies for more conductive organic electronic devices.

Reference and notes

[1] G. Gryn'ova, C. Corminboeuf, *J. Phys. Chem. Lett.* **2016**, *7*, 5198-5204.
[2] G. Gryn'ova, C. Corminboeuf, *J. Phys. Chem. Lett.* **2018**, *9*, 2298-2304.