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Electronic States and Electronic Coupling in Organic Molecular Systems[1]

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The understanding of electronic transport in organic molecular systems is at an early stage. The systems of interest range from crystals and thin films with well defined bulk transport to the limit of single molecule devices where the source and drain electrodes are integral to the transport processes. Nonetheless there are several important factors that are shared among these different systems, including frontier electronic energy level alignment, electronic coupling and structural reorganization or vibrational coupling. In this talk, the electronic coupling and energy level alignment for several prototypical systems will be presented, based on self consistent first principles calculations. The goal is to understand the relationship between molecular structure, the binding of the molecules to each other or to a metal contact and the electronic coupling that is developed among the frontier states that support transport. For intermolecular coupling in organic molecular crystals, the impact of structure on electronic coupling has been analyzed by comparing the energy bands in derivatized acenes that form crystals with different packing motifs. In the case of single aromatic molecules on metal contacts, several link chemistries have been studied. One of the themes that emerges from these studies is that the electronic coupling pertinent for transport plays a minor role in the binding of the system. This poses a significant challenge in the search for molecular systems with improved transport characteristics.

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