



Molecular design of semi-conducting metal-organic framework films

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Abstract:

Electronic properties of organic semiconductors (OSC) highly depend on the structural assembly of molecules and their vibrational flexibility in a material. These determine the microscopic intercommunication between the electronically active sites, resulting in a materials conduction. In most cases, aggregation of OSC is hard to control and a multitude of assembly possibilities occurs. Here, we have employed a metal-organic framework (MOF) type of crystalline assembly strategy to engineer the arrangement of the spiropyran photoswitches and functionalized pentacene-based semiconductors incorporated at controlled positions with defined intermolecular distances in MOFs, and demonstrated the change of the electronic and spectroscopic properties of molecules and films towards assembly in the spatially ordered MOF structure.

Based on our previous proof-of-principle study on spiropyran embedded in MOFs [1], showing for the first time the remote switching of the electric conduction of a MOF material, we used the combination of quantum mechanics and molecular mechanics approaches to design new MOF candidates with conductance properties that can be reversibly changed by light. With the implemented temperature-dependent dynamics of the molecules in a material, the charge carrier mobilities, considering both band-like transport and the Marcus charge hopping were obtained. A thorough quantum mechanical investigation allows identifying localized frustrated rotations of the pentacene cores as the reason for the breakdown of band transport [2]. It gives perspectives for realization of the highly anisotropic conduction with oriented photosensitive conduction highways.

References and acknowledgements

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