

Tunable electronic properties of self-assembled donor-acceptor monolayers on metal surfaces

Interviene:

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In novel organic optoelectronics applications, the device efficiency depends crucially on the energy barrier that controls charge carrier injection at molecule/electrode interfaces. These processes are determined by the chemical interaction between the deposited species and the inorganic surface, as well as on morphological and structural aspects. One possible strategy to further steer the structural and electronic properties at interfaces is to use molecular mixtures such as donor-acceptor molecular pairs, since the introduction of the supramolecular interaction may have an influence on the molecule-substrate interaction. The accurate understanding of the intermolecular and molecule-substrate interactions, as well as of the interplay among them, is therefore a fundamental step for designing the functionality of the self-assembled system.

Within this framework, we use a powerful combination of surface sensitive techniques to determine the structure, the energy level alignment and interfacial charge transfer of two-dimensional donor-acceptor monolayers in direct contact with noble metal (111) surfaces. We show that the formation of an ordered mixed layer with a maximized donor-acceptor contact area leads to a characteristic energy level alignment at the molecule/metal interface regardless of the particular molecules and substrate [1]. We also provide evidence that the deposition of two different molecular species modifies the molecule's adsorption height, with relevant effect on the interfacial energy barrier as well on the chemical bonding with the metal surface [2]. Finally, we demonstrate that, by appropriate design of the supramolecular environment, charge transfer into empty molecular levels can be triggered across the metal-organic interface without the need to intercalate substrate-functionalizing buffer layers [3].

[1] El-Sayed, P. Borghetti, et al. *J. Phys. Chem. C*, 116 (2012) 4780.

[2] E. Goiri, M. Matena, A. El-Sayed, J. Lobo-Checa, P. Borghetti, C. Rogero, B. Detlefs, J. Duvernay, J. E. Ortega, D. G. de Oteyza, *Phys. Rev. Lett.*, 112 (2014) 117602

[3] P. Borghetti, A. El-Sayed, E. Goiri, C. Rogero, J. Lobo-Checa, L. Floreano, J. E. Ortega, and D. G. de Oteyza, *ACS Nano*, 8 (2014) 12786

Seminario

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