

A DFT study on the interface of prototype organic semiconductors and the silver surface

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Abstract:

One of the most important factors that affect the performance and efficiency of organic electronic devices are the metal/organic interfaces. In this work, we employ first-principles Density Functional Theory (DFT) calculations in order to investigate the structural and probe the electronic properties of prototype organic materials (i.e. P3HT and PC₆₀BM) in the proximity of Ag. First, we examine the energetic stability of various conformations for the adsorption of PC₆₀BM on Ag(111) surface, depending on the position of PC₆₀BM's functional group. We also investigate the preference on the coverage rate of PC₆₀BM on the silver surface. Furthermore, we calculate the charge rearrangement at the interface and the respective interfacial dipole that is formed due to adsorption. We use the interfacial dipole, together with the intrinsic dipole of the adsorbed molecule to assess the total electrostatic potential step across the system. For the case of crystalline P3HT, the preferred adsorbed geometry is with the thiophene backbone parallel to the Ag surface. Results presented here, show that by controlling the adsorption details at the metal/organic interface, the charge rearrangement is modified and influences the energy level alignment of the different layers of the device.