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TÉMA

Structural and electronic properties of PTCDA organic molecules on semiconductor surfaces

Nicoleta Nicoara

Dept. of Condensed Matter Physics, Universidad Autónoma de Madrid

The possibility to integrate organic molecular semiconductors as active components in conventionally used inorganic semiconductor-based devices represents nowadays an active and rapidly expanding research field. The increased reactivity of semiconductor surfaces limits in many cases the formation of well ordered layers, therefore detailed knowledge related to the bonding, interaction strength, and molecular ordering are required in order to understand the processes which occur at the molecules-substrate interface.

By means of scanning tunneling microscopy (STM) under ultra-high vacuum (UHV) we investigate the adsorption and electronic properties of a prototype organic molecule PTCDA (3,4,9,10 perylene tetracarboxylic dianhydride) on semiconductor substrates with different reactivities: clean Si(111)-7×7 and Sn "passivated" Si(111) surfaces. Particular emphasis is given to the interface formation, which is directly influenced by the substrate properties and which plays a crucial role in the molecular ordering and the electronic properties of the organic molecules.

The visualization of PTCDA molecular orbitals in bias-dependent high resolution STM images allows us to elucidate the adsorption site and bonding configuration and indicates a possible charge transfer. A fine balance between intermolecular and molecule-substrate interactions favors and stabilizes the formation of quasi one-dimensional PTCDA chains on Si(111)-(2√3 × 2√3)R30°Sn surface, in contrast to a random adsorption of molecules on the more reactive Si(111)-7×7 substrate.

In the last case, the interpretation of experimental STM images is not straightforward. Complementary density-functional theory (DFT) calculations and simulated STM images with realistic tips are necessary to understand the complex splittings and shifts of molecular orbitals. These splittings can be understood under symmetry and charge transfer arguments, which characterize a strong partially-ionic covalent bonding involving the carbonyl groups of PTCDA and silicon dangling bonds.

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