A donor-acceptor complex on the surface of a metal

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Resumen

TTF-TCNQ is a prototypical molecular metal, well known in the field of molecular organic materials by its bulk quasi-one dimensional electronic structure. Donor-acceptor interactions play an important role in the crystal formation. Charge transfer between π-stacked molecular chains of the donor and the acceptor species give rise to one dimensional electron and hole bands along the stacking direction. In spite of the large number of studies focused on the bulk properties of TTF-TCNQ salts, very little is known about the donor-acceptor interactions and the electronic structure of the compound on the surface of a metal.

Here we report on the persistence of donor-acceptor interactions in TTF-TCNQ films adsorbed on a Au(111) surface, and their role on interfacial properties from a local perspective. The study has been carried out by a combination of Low Temperature Scanning Tunneling Microscopy (STM)/spectroscopy (STS) measurements, and Density Functional Theory (DFT) calculations.

As individual components, TTF and TCNQ exhibit very distinct bonding properties with the metal surface. TTF chemisorbs on Au(111) donating charge to the surface. Repulsive long range interactions between the positively charged molecules lead to the stabilization of a quasi-periodic lattice of spaced monomers. TCNQ is physisorbed on Au(111) and does not exhibit any charge transfer to the surface.

Co-adsorption of TTF and TCNQ gives rise to a spontaneous formation of mixed TTF-TCNQ domains driven by donor-acceptor interactions. The molecules self-assemble in rows, resembling the bulk structure. However, they exhibit a planar adsorption configuration at the surface. As a consequence of this arrangement, the metal-organic interface shows metal-like bands with hybrid molecular and metallic surface character.