Study of the structural and electronic properties of TTF-TCNQ on Cu(111)

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Organic molecule-metal interfaces are model systems for studying molecular self-assembly and charge-transfer phenomena[1]. This work investigates the structural, chemical, and electronic properties of the electron-donor tetrathiafulvalene (TTF) and the electron-acceptor tetracyanoquinodimethane (TCNQ), deposited on Cu(111) under ultra-high vacuum (UHV) conditions. The structure of the deposits was characterized by low-temperature scanning tunneling microscopy (STM), while their chemical and electronic properties were investigated using X-ray and ultraviolet photoelectron spectroscopy (XPS and UPS).

Several ordered TCNQ phases were identified on Cu(111), with the self-assembly process showing a strong dependence on substrate temperature and molecular coverage[2]. STM observations suggest that interactions between cyano groups play a role in stabilizing the molecular assemblies. In contrast, TTF exhibits a stronger interaction with the substrate, limiting its surface diffusion and favoring the formation of local structures[3]. XPS and UPS measurements reveal, for TCNQ/Cu(111), electron transfer from the copper substrate to the first molecular layer, leading in particular to partial occupation of the LUMO. For TTF, the results suggest a strong interaction with copper, potentially associated with partial molecular dissociation. Finally, several mixed TTF–TCNQ phases were observed, some of which exhibit a 1:1 stoichiometry comparable to those reported on other metal substrates[1,4]. These results highlight the decisive influence of molecule–substrate interactions on the structural organization and electronic properties of donor-acceptor molecules on metal surfaces.

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