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First principles study of aromatic molecules on Copper substrates

ANDREA FERRETTI, Physics Department, University of Modena and Reggio E., and Natl Center S3-INFM-CNR, Modena, Italy, ARRIGO CALZOLARI, ROSA DI FELICE, Natl Center S3-INFM-CNR, Modena, Italy, ALICE RUINI, ELISA MOLINARI, Physics Department, University of Modena and Reggio E., and Natl Center S3-INFM-CNR, Modena, Italy — Conjugated molecules and oligomers have attracted large attention in the last years due to their interesting electronic and transport properties. The interaction of these molecules with metallic surfaces is attractive both for the properties of the metal-organic interface and for the possibility of tuning the crystal structure of the films using the surface as a template. In the present work we focus on an ab initio investigation based on density functional theory of pentacene adsorbed on Copper surface. We also compare with the case of the DPDI molecule adsorbed on the same substrate. We address structural and electronic properties, and we relate our results to experimental data, STM, XSW, and angle resolved photoemission spectroscopy in particular. Our theoretical findings show a flat adsorption geometry for both pentacene and DPDI molecules. For what concerns the electronic structure, a strong rehybridization of the molecular electron states is found in the range of the occupied π states. These results lead to an interpretation of the adsorption mechanism of pentacene in terms of a coupling intermediate between the physi- and the chemi-sorption regimes.

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