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A theoretical and experimental investigation on the adsorption of pentacene on the Cu(322) surface JERONIMO MATOS, University of Central Florida, MICHELE SAUVAGE-SIMKIN, Synchrotron SOLEIL and UR1-CNRS, ALESSANDRO COATI, Synchrotron SOLEIL, YVES GARREAU, Synchrotron SOLEIL and Universite Paris Diderot, ALINA VLAD, Synchrotron SOLEIL, KATHRIN MULLER, Max Planck Institut fr Festkrperforschung, AZZEDINE BENDOUNAN, Synchrotron SOLEIL, ABDELKADER KARA, University of Central Florida — In this study, complementary techniques including density functional theory (DFT), grazing incidence x-ray diffraction (GIXD), and scanning tunneling microscopy (STM) are used to study the surface distortions induced by the adsorption of pentacene on the stepped Cu(322) surface. GIXD measurements are performed for the clean Cu(322) surface and at various coverages of pentacene, up to one monolayer. For the one monolayer case, reciprocal space maps from GIXD measurement suggest the reconstruction of the steps to double the step width and height, with two pentacene molecules present at each terrace. Complementary DFT calculations are carried out, with and without the self-consistent inclusion of vdW interactions, using the optB88-vdW and PBE functionals. Our investigation illustrates a prototype method for conducting future benchmarking studies to assess the accuracy of the current self-consistent vdW functionals when applied to organic molecule adsorption.

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