

Abstract Submitted
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Adsorption of pentacene on (100) vicinal surfaces: role of coordination, surface chemistry and vdWs effects¹ JERONIMO MATOS, ABDELKADER KARA, University of Central Florida — In contrast to low miller index surfaces, vicinal surfaces are characterized by steps and step edges that not only present an interesting atomic landscape for the adsorption organic molecules, but also a unique electronic structure resulting in part from the low coordinated atoms at the step edges. The adsorption of pentacene on the stepped (511), (711), (911) surfaces (respectively 3, 4 and 5-atom wide terraces) of Cu and Ag (coinage transition metals); Pt (reactive transition metal); and Ni (reactive, magnetic transition metal) are studied using density functional theory, in order to investigate the support effects arising from differing surface chemistry. We compare the adsorption energy, adsorption geometry and electronic structure predicted by the PBE functional with those obtained from one of the optimized vdW-DF methods: optB88-vdW.

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