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Pentacene on Cu(911): A Density Functional Theory study ABDELKADER KARA, University of Central Florida — I use density functional theory to calculate the adsorption energies, geometric and electronic structures of pentacene ($C_{22}H_{14}$) on the Cu(911) vicinal surface. The pentacene molecule is found to adsorb nearly flat (slightly arched at the edges) on top of the terrace but close to the step with an adsorption energy of 1.3 eV. The adsorption geometry on Cu(911) is found to differ from that of on Cu(110); but there is a strong bonding between the center carbon atoms of the molecule and Cu atoms near the step. In accord with experimental observations, the arched geometry induces brightness at the edges of the molecule in the STM images. The alignments of the energy levels at the interface induce a change in the work function of about -0.4 eV, in qualitative agreement with the observed -0.9 eV, which is an indication of charge transfer from the molecule to the surface. The details of the electronic structure at the interface will be presented.

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