Abstract Submitted
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Electronic Structure and adsorption of Pentacene on Cu and Ag (110).[1] ABDELKADER KARA, Department of Physics, University of Central Florida, Orlando FL32816 — The adsorption of pentacene ($C_{22}H_{14}$) at coverages of one and 0.8 monolayer on Ag(110) and Cu(110) is studied using density functional theory. The unit cells for these systems are 6x2 and 7x2 for Ag(110) and Cu(110), respectively. The pentacene molecule adsorbs nearly flat (with a structural corrugation of about 0.6) at a position 2.5 above the surface. On Ag(110), the adsorbed pentacene is even flatter (0.45 corrugation) and sits higher (about 2.8) then the case of Cu. On Cu(110), most of the carbon atoms adsorb on top of Cu atoms, which is not the case on Ag(110). The resulting changes in the electronic states and the nature of the bonding will be discussed and comparison between the two systems will be presented.

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