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Chemisorption of Anthracene on Cu(110) JERONIMO MATOS, ABDELKADER KARA, University of Central Florida — We use density functional theory (PBE) to calculate the adsorption of an Anthracene molecule on Cu(110). Anthracene adsorbs at a height of 2 Å above the surface and has a binding energy of 562 meV/molecule. We also found noticeable changes in the atomic and electronic structures of both the molecule and the substrate. The molecule is bent while the surface atoms experience a buckling. The dz^2 state of the copper atoms that are directly under carbon atoms presents new states near the Fermi level. These effects, in addition to a change in the work function, classify this system as chemisorption. We also determined the barrier for diffusion along the Cu(110) channel to be 77 meV.

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