

Abstract Submitted
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Chemisorption of Guanine on Cu(110) JERONIMO MATOS, ABDELKADER KARA, University of Central Florida — We use density functional theory (PBE) to calculate the adsorption of a guanine molecule on Cu(110). At saturation coverage, guanine adsorbs tilted with the oxygen atom strongly bound to one of the surface atoms at a height of 2.12 Å above this surface atom with a binding energy of 430 meV/molecule. The substrate top layer atoms show a buckling of 0.22 Å, while the molecule experiences a twist from the flat configuration in the gas phase. The dz^2 state of the copper atom -that is bound to the oxygen atom- presents an enhancement in its density near the Fermi level. We calculated a drop in the work function of 0.34 eV upon adsorption of guanine on Cu(110). These effects classify this system as chemisorption.

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