Adsorption Characteristics of Acenes on Cu(110) and Ag(110)

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Using density functional theory and the generalised gradient approximation, we have calculated the adsorption characteristics of five acenes (Benzene, Naphtalene, Anthracene, Tertracene and Pentacene) on the (110) surface of copper and silver. We found the binding energy to increase with number of carbon atoms in the molecule for both silver and copper cases. However, the increase in the binding energy is substantially large for the case of copper as compared to the case of silver. In the case of adsorption on Ag(110), all geometrical and electronic structural changes point to physisorption for all acenes, while for the adsorption on Cu(110), these characteritics show a gradual shift from physisorption (from Benzene to Naphtalene) to chemisorption for Tetracene and Pentacene with the border case of Anthracene. The characteristics to distinguish between physisorption and chemisorption used in the present study are: bending and tilting of the molecule, buckling in the substrate top-most layers, charge transfer, change in the workfunction, d-band center and width, and finally the existence of interface states near the Fermi level.

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