

# Adsorption of Co- and Cu-phthalocyanines on Au(100) surfaces

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In order to develop and improve the performance of organic based electronic devices, an extended and comprehensive understanding of the basic physics which appears at the interface between organic and metallic materials is required. We present a density functional theory study of the structures of (metal-)phthalocyanines on a Au(100) surface. The centre atom of the phthalocyanine-molecule can be replaced by a relatively large number of different atoms in order to design the molecule's electronic properties. In this work, we primarily study the Cobalt phthalocyanine (CoPc) and Copper phthalocyanine (CuPc). The induced charge densities, and the x-ray adsorption spectra (XAS) have been calculated using the Quantum Espresso packages. We investigate how these phthalocyanines arrange themselves in monolayers, double and triple layers and higher multiples. Starting from a third layer, Cu-centered molecules tend to form one or two buried layers of flat lying molecules, while the topmost molecular layer is standing up. This behaviour is not observed in the Co-centered molecules, which can be traced back to the half occupied d-orbitals of the molecules, which lie in plane for Cu-centered molecules, but reach out of plane for the Co-centered molecules, thereby offering different intermolecular binding arrangements. Our theoretical results are compared to experimental data [1].

References:

[1] F. Petraki, H. Peisert, I. Biswas, T. Chasse, J. Phys. Chem. C 2010, 114, 17638-17643