

# Formation of thin organic layers at the example of Co- and Cu-Phthalocyanines on Au-substrates – a theoretical investigation

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## Abstract

Phthalocyanines (Pc) with or without a metal center are currently under intense investigation in surface physics. The biocompatibility of these molecules together with their chemically tunable electronic structure makes them for instant highly interesting for energy transfer processes in medical applications. Furthermore, in nanotechnology, they are especially useful due to their flexibility, since the basis of these molecules, i.e. the porphyrin core, can easily be varied with different functional groups substituting parts of the molecule or simply attached to the core of the molecule. Upon exchanging the center atom, the binding energy to a substrate, the molecular deformation or the spin state can be tailored.

In this work, we present our first principles investigations of Co-Pc and Cu-Pc on Au(100)-surfaces. In contrast to our previous studies on tetraphenyl porphyrins on Au(111) [1,2] or metal-free phthalocyanines on Au(110) [3], the flat surface geometry of Au(100) does not induce the strong deformations we observed for these cases. A comparatively strong interaction of the complete molecule with the substrate is observed. In our work, we investigated high coverage structures as a first step towards the organic/inorganic interface as is useful for organic electronic devices.

Taking the next steps, we moved on towards the formation of multiple molecular layers.

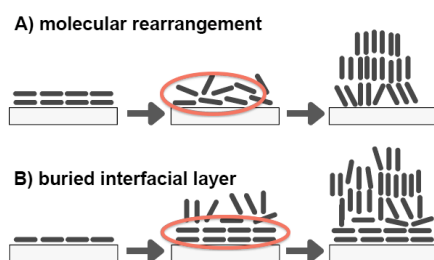
In experiment, a structural transformation is observed, with the molecules lying flat in the beginning and moving to a standing arrangement for higher Pc film thicknesses. Experiments give a hint that a buried interface structure is formed, the structure of which we address by our calculations. A variety of two-, and three-layer thick molecular adsorbates have been investigated.

While simulated STM-images do not uniquely resolve the number of layers below, the density of states shows some characteristic shifts, especially of the d-orbitals at the Co-center.

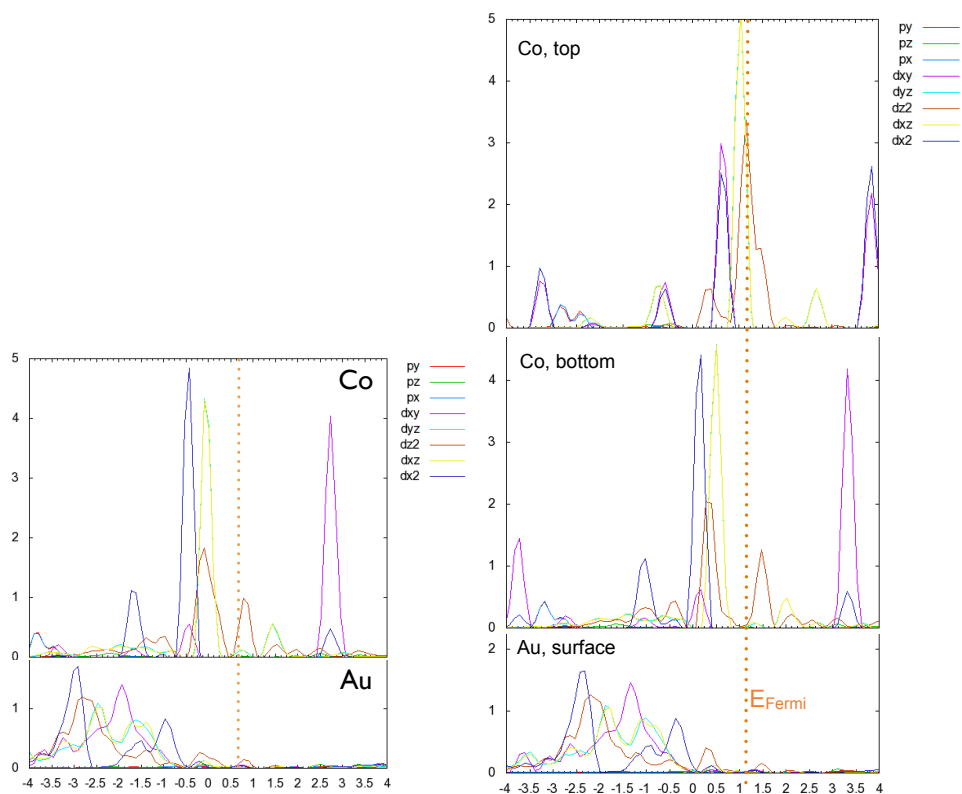
## References

- [1] S. Muellegger, E. Rauls, et al. ACS Nano 5, 6480 (2011).
- [2] S. Müllegger, M. Rashidi, T. Lengauer, E. Rauls, W. G. Schmidt, G. Knor, W. Schöfberger, and R. Koch, Phys. Rev. B 83 , 165416, (2011).
- [3] E. Rauls, W.G. Schmidt, T. Pertram, K. Wandelt, Surf. Sci. 606, 1120, (2012).

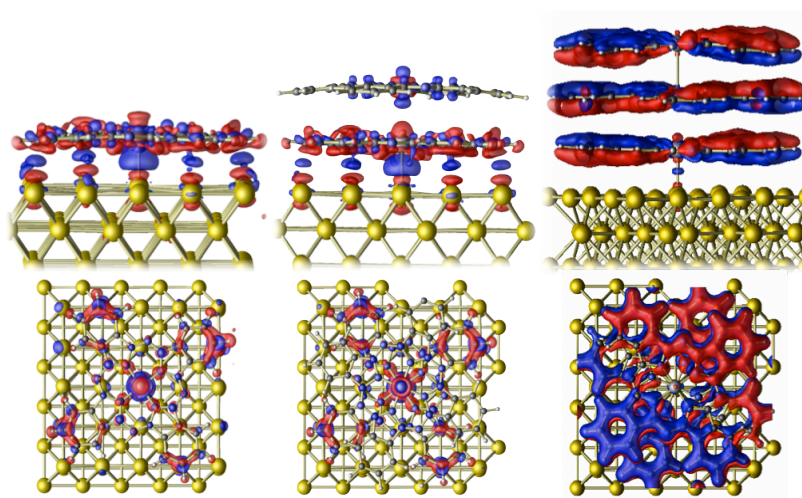
## Figures



**Fig. 1: Schematic representation of the formation of multiple molecular layers**



**Fig. 2: State-decomposed density of states at the Co-center of Co-Pc-molecules in a single layer (left) or a double layer (right) of molecules**



**Fig. 3: Calculated charge density differences upon adsorption of 1, 2, or 3 Co-Pc molecules on a Au(100) surface**