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S E M I N A R
aus
Halbleiterphysik und Nanotechnologie

Di, 30.5.2017, 13:00 Uhr, Hörsaal für Physik

"Characterization of the interface geometry of organic adsorbates"

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The geometric structure of organic adsorbates on dielectric or metallic substrates is one of the most important piece of information about such interfaces as it determines many of its physical properties. In this presentation we will show how total energy calculations within the framework of van-der-Waals corrected density functional theory (DFT) may contribute to the understanding of the adsorption behaviour of rod-like organic molecules on such substrates. In particular, the growth directions of epitaxially grown, highly ordered, needle-like crystalline networks of parahexaphenyl on ultra-thin hexagonal boron nitride is analyzed in terms of atomic force microscopy supported by such DFT calculations [1].

The second part of the presentation will focus on the adsorption of nickel tetra-phenyl porphyrin on the Cu(100) surface. We will present a comprehensive characterization of the geometrical and electronic structure utilizing DFT as well as scanning tunneling microscopy and photoemission tomography, where the result of angle resolved photoemission spectroscopy measurements are systematically compared to the Fourier Transform of molecular orbitals, obtained within DFT. As we will show, photoemission tomography not only allows for a direct assignment of peaks in the angle integrated photoemission spectrum to individual molecular orbitals but also for the characterization of the azimuthal alignment of the molecules [2]. As such, our results emphasize that a multi- technique approach is essential in order to have a complete picture of the adsorption behavior of such organic molecules on dielectric or metallic substrates.

[1] A. Matković et al., *Scientific Reports* **6**, 38519 (2016)
[2] G. Zamborlini et al., submitted (2017)