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Electronic and geometric structure of organic overlayers from angle-resolved UPS and DFT calculations — •Matus Milko[1], Sophia Huppmann[2,3], Markus Scholz[2,3], Wiessner Michael[2,3], Achim Schöll[2,3], Friedrich Reinert[2,3], and Peter Puschnig[1] — [1]Chair of Atomistic Modelling and Design of Materials, Montanuniversität Leoben, Austria — [2]Experimentelle Physik VII und Wilhelm Conrad Roentgen Research Center for Complex Material Systems, Universität Würzburg, Germany — [3]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, Germany

We present a combined experimental and theoretical study on the electronic and geometric structure of metal-free phthalocyanine (H_2Pc) and copper phtalocyanine (CuPc) adsorbed on Au(110). Experimentally, mono-layers of the molecules were analyzed by low energy electron diffraction (LEED) revealing ordered superstructures. Then, angular resolved photoelectron spectroscopy (ARPES) was employed to examine the valence electronic structure. Theoretically, we computed the electronic structure within the framework of density functional theory corrected for many body effects which leads to correct ordering of orbitals. Moreover, using ARPES orbital maps of the highest occupied molecular orbitals in reciprocal space were obtained which we could directly compare to our *ab initio* results. We demonstrate, how one can extract information about the azimuthal orientation of the molecules on the substrate by this approach. Thus in combination with LEED we can provide a complete two-dimensional structure determination.

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