

Abstract Submitted
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Electronic Structure of CoPc Adsorbed onto Ag(100): Evidence for Molecule-Substrate Interaction Mediated by Co-3d Orbitals ERIC SALOMON, Aix-Marseille University, France, PATRICK AMSALEM, Humboldt University, Berlin, Germany, NOA MAROM, The University of Texas at Austin, MARTIN VONDRACEK, Institute of Physics AS CR, Czech Republic, LEEOR KRONIK, Weizmann Institute of Science, Israel, NORBERT KOCH, Humboldt University, Berlin, Germany, THIERRY ANGOT, Aix-Marseille University, France — The electronic structure of cobalt-phthalocyanine (CoPc) molecules adsorbed on Ag(100) is investigated by photoemission spectroscopy. The results are compared to first principles electronic structure calculations, based on many-body perturbation theory in the GW approximation. The photoemission data, obtained from both multilayer and monolayer films of CoPc, show that charge-transfer occurs between the first molecular layer and the metal surface. Varying the photon energy, to tune the photoionization cross sections, reveals that the charge-transfer related interface states mainly involve the Co-3d atomic orbitals of the Co central atom. GW calculations for the neutral CoPc molecule and its anion compare well with the experimental observations for a multilayer and a monolayer CoPc film, respectively. They confirm the major role played by the Co atom in the charge transfer process and elucidate the complex energy rearrangement of the molecular electronic levels upon adsorption on the metal.

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