

O 100: Organic electronics and photovoltaics

Time: Friday 11:15–12:30

Location: WIL B122

O 100.1 Fri 11:15 WIL B122

Spin-resolved photoemission study of the interface of transition metal phthalocyanines (CuPc, FePc, CoPc) on Co(100)

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Because of their unpaired electrons the three transition metal phthalocyanines (MePcs) CuPc, FePc and CoPc are promising candidates for the development of molecular spintronics devices based on organic-inorganic hybrid systems. For these future devices the injection of spin-polarized electrons is necessary. Therefore the interface between a ferromagnetic contact material and the organic layer plays a major role for the performance of the device.

In this study the electronic and magnetic properties of the interface between the ferromagnetic cobalt and the metal-organic molecules CuPc, FePc and CoPc were investigated by different means of ultraviolet photoelectron spectroscopy (UPS). Ultrathin MePc films were grown in situ on Co(100) under ultra high vacuum conditions. These were studied by spin-integrated and spin-resolved UPS. Linear dichroism with unpolarized light was used to examine the valence band structure. These studies show that all molecules interact with the cobalt substrate so that new states occur which are located at the interface. They also show that the interaction of FePc and CoPc with the Co substrate is similar to each other but differs from the interaction of CuPc with Co.

O 100.2 Fri 11:30 WIL B122

Smooth growth of organic semiconductor films on graphene for high efficiency electronics— ●GREGOR HLAWACEK^{1,2}, FAWAD S. KHOKHAR¹, RAOUL VAN GASTEL¹, BENE POELSEMA¹, and CHRISTIAN TEICHERT² — ¹Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, NL-7500AE, Enschede, The Netherlands — ²Institute for Physics, University of Leoben, Franz Josef Str. 18, A-8700 Leoben, Austria

High quality thin films of conjugated molecules with smooth interfaces are important to assist the advent of organic electronics. Here, we report on the layer-by-layer growth of the organic semiconductor molecule para-sexiphenyl on the transparent electrode material graphene. State of the art Low Energy Electron Microscopy, micro Low Energy Electron Diffraction and spot profile analysis techniques revealed the morphological and structural evolution of the thin film. Subtle difference in the molecular arrangement in comparison to graphite are confirmed by molecular dynamics simulations. Initial islands are found to have a meta stable structure that is characterized by flat lying molecules. With increasing coverage this structure changes into a herringbone arrangement similar to the {111} bulk layer. The layer-by-layer growth of 6P on graphene proceeds by subsequent adding of {111} layers.

O 100.3 Fri 11:45 WIL B122

Elucidation of Partial Charge Transfer from the Methoxy Groups of Substituted Pyrene as Donor in Complexes with Tetracyanoquinodimethane— ●KATERINA MEDJANIK¹, SERGEJ NEPIJKO¹, HANS-JOACHIM ELMERS¹, GERD SCHÖNHENSE¹, PETER NAGEL², STEFAN SCHUPPLER², DENNIS CHERCKA³, MARTIN BAUMGARTEN³, and KLAUS MÜLLEN³ — ¹Ins. für Physik, Johannes Gutenberg-Universität, Mainz — ²Karlsruhe Institute of Technology, ANKA — ³Max-Planck Ins. for Polymer Research, Mainz

Novel charge transfer (CT) compounds can be synthesized on the basis of large polycyclic aromatic hydrocarbons [1]. Microcrystals of the CT-compounds tetra- and hexamethoxypyrene/tetracyanoquinodimethane (TMP_x/HMP_x-TCNQ_y) in different stoichiometries $x : y = 1 : 1$, $1 : 2$ and $2 : 1$ were grown from solution via vapour diffusion. These crystal-

lite fractions were studied by NEXAFS with particular emphasis on direct fingerprints of a charge transfer. Oxygen and nitrogen K-edge NEXAFS gives direct access to the unoccupied orbitals in the donor and acceptor, respectively. With increasing HMP content, a strongly rising O 1s pre-edge signal comes along with a substantial drop of N 1s resonance intensity. Charge is transferred from the π^* -orbital of the methoxy-group to the σ^* -orbitals b_{1g} and b_{2u} and - to a weaker extent - to the π^* -orbitals b_{3g} and a_u of the cyano-group of TCNQ, particularly strong for the 2:1 compound. Funded by DFG/TR49, Graduate School of Excellence MAINZ, Centre of Complex Materials COMATT.

[1] K. Medjanik *et al.*, Phys. Chem. Chem. Phys. **12**, 7184 (2010)

O 100.4 Fri 12:00 WIL B122

Tuning the hole-injection barrier at the organic-metal interface with a strong organic acceptor— ●JENS NIEDERHAUSEN¹, PATRICK AMSALEM¹, JOHANNES FRISCH¹, ANDREAS WILKE¹, BENJAMIN BRÖKER¹, ANTJE VOLLMER², RALPH RIEGER³, KLAUS MÜLLEN³, JÜRGEN P. RABE¹, and NORBERT KOCH¹ — ¹Humboldt-Universität, Institut für Physik, Berlin, Germany — ²Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — ³Max Planck Institut für Polymerforschung, Mainz, Germany

Ultraviolet photoelectron spectroscopy was used to investigate how pre-adsorption of the strong electron acceptor hexaazatriphenylenehexanitrile (HATCN) on Ag(111) affects the energy level alignment of two subsequently deposited conjugated organic materials (COM). The tuning of the sample work function (WF) by precovering Ag(111) with HATCN monolayers oriented either in a lying or in a standing fashion is found to induce important variations in the hole injection barrier (HIB) of the COM. An interface dipole of similar magnitude is observed upon adsorption of both COM overlayers on a lying HATCN monolayer with low WF. It is related to the push-back effect, which occurs at specific adsorption sites of the molecules at very low coverage. For COM adsorbed on Ag(111) precovered with a standing HATCN monolayer with high WF, Fermi level pinning is identified in both cases, and appears as a fundamental limit to further HIB lowering. The observed behavior is reminiscent of the adsorption characteristics of COM on high WF conducting polymer substrates. This leads to a situation where the HIB decreases by up to 1.1 eV.

O 100.5 Fri 12:15 WIL B122

Experimental and theoretical spin-resolved investigations of the electronic structure of open shell metal-phthalocyanines.

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The valence band structure of different metal-phthalocyanines (MePcs) was investigated by comparison of gas-phase ultraviolet photoelectron spectra (UPS) and spin-resolved thin film UPS spectra with simulated spectra calculated using density functional theory (DFT). High resolution gas phase UPS spectra of cobalt phthalocyanine (CoPc) and iron phthalocyanine (FePc) show states which were unresolved in earlier studies. They were compared to Kohn-Sham eigenvalue spectra, derived from unrestricted DFT calculations. The composition of the molecular orbitals (MOs) just below the highest occupied molecular orbital (HOMO) was studied using UPS thin film spectra recorded at different excitation energies and thus different cross sections for s-, p-, and d-orbitals. Further the spin polarization of these MOs was derived from the DFT calculations and compared to thin film spin-resolved UPS spectra. The combination of these methods leads to a detailed image of the ground state electron system configuration with new insights into the behavior of the spin system.