

DS 35: Organic thin films III: Monolayers and crystals

Time: Thursday 17:45–19:30

Location: H 2032

DS 35.1 Thu 17:45 H 2032

Dithiocarbamate Monolayers for Noble Metal Surface Functionalization — •TOBIAS SCHÄFER¹, PHILIP SCHULZ¹, CHRISTIAN EFFERTZ¹, DANIEL GEBAUER¹, DOMINIK MEYER¹, RICCARDO MAZZARELLO², and MATTHIAS WUTTIG¹ — ¹I. Institute of Physics (IA), RWTH Aachen University — ²Institute for Theoretical Solid State Physics, RWTH Aachen University

Organic electronic devices like organic light emitting diodes (OLED), photovoltaics (OPV) and thin-film transistors (OTFT) are well-known for their potential in the field of optoelectronics. Yet a significant improvement in device functionality is expected by tailoring the interface between metal electrode and the functional organic film. One approach is to modify the electrodes by self-assembled monolayers (SAMs).

Here, we present a combined experimental and theoretical investigation of dithiocarbamate (DTC) monolayers on noble metal surfaces. The monolayer systems were investigated by photoelectron (PES) and infrared spectroscopy (FT-IR) which show densely packed DTC films heading to very low work functions. The pronounced alignment of the electronic structure can be reproduced well by density functional theory (DFT). Thereby the low work function is explained by the formation of strong bond dipoles, intrinsic molecular dipoles and the high packaging density of the molecules. The superior electronic coupling between metal electrode and active organic layers was shown in an OTFT geometry. Thus, we present a promising and reliable route towards low work function metal contact interfaces to n-type and ambipolar organic transport layers.

DS 35.2 Thu 18:00 H 2032

Organic heteroepitaxy of PTCDA and SnPc on single crystalline silver — •MARCO GRUENEWALD, KRISTIN WACHTER, FALKO SOJKA, MATTHIAS MEISSNER, ROMAN FORKER, and TORSTEN FRITZ — University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

Here we report on the interaction mechanisms at metal-organic and organic-organic interfaces in heterostructures of highly-ordered ultrathin layers of the dye molecules 3,4,9,10-perylene-tetracarboxylic dianhydride (PTCDA) and tin(II)-phthalocyanine (SnPc) on Ag(111). The thin films were characterized optically by in situ Differential Reflectance Spectroscopy (DRS), followed by an extraction of the related optical constants.

For the first monolayer PTCDA and the first monolayer SnPc the well-known covalent interaction [1] between adsorbate and substrate is manifested in broad and structureless absorption spectra. Further layers of PTCDA and SnPc, however, are efficiently optically decoupled from the first monolayer. Hence, a monomer signature for the respective molecules is observed until aggregation occurs. In the first monolayer of PTCDA on top of a SnPc monolayer film the coexistence of neutral and anionic PTCDA is concluded. Furthermore, SnPc on top of a PTCDA and on top of a SnPc monolayer was investigated optically. Accordingly, the existence of a PTCDA interlayer induces a highly-ordered growth of SnPc up to several monolayers.

REFERENCES

- [1] M. Häming et al., Phys. Rev. B 82, 235432 (2010).

DS 35.3 Thu 18:15 H 2032

A systematic study on fluorination: Rubrene and its fluorinated derivatives — •FALK ANGER¹, EVELYN ADAMSKI¹, KATHARINA BROCH¹, ALEXANDER GERLACH¹, TOSHIYASU SUZUKI², and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — ²Institute for Molecular Science, Myodaiji, Okazaki 444-8787, Japan

A promising way to modify the electronic levels of organic semiconductors is partial or complete fluorination. Rubrene (C₄₂H₂₈) has been shown to be a suitable semiconductor for applications, for which numerous experimental efforts have been done. In this study, we present thin films of partly (C₄₂H₁₄F₁₄) and completely (C₄₂F₂₈) fluorinated rubrene. For the first time we investigated thin films of these materials grown on a native SiO₂ substrate using optical spectroscopy, complementary X-ray reflectivity and AFM. The materials grow to a large extent amorphously and exhibit a smooth surface. However, depending on the growth parameters the molecules can form ordered, dendritic structures that extend on a micrometer scale. The variation

of the HOMO-LUMO transition with fluorination is discussed.

- [1] M. Kytka et al., J. Chem. Phys. **130**, 214507 (2009)
[2] S. Kowarik et al., Phys. Chem. Chem. Phys. **8**, 1834-1836 (2006)

DS 35.4 Thu 18:30 H 2032

3h-Auger decay in the π -band of HOPG — •MATTHIAS RICHTER, DANIEL FRIEDRICH, and DIETER SCHMEISSER — Brandenburg University of Technology Cottbus, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

In this contribution we report on the electronic structure of highly oriented pyrolytic graphite (HOPG). HOPG is a model system because of the clear separation between π - and σ -bands in the valence band regime. X-ray based measurements were done at the U49/2-PGM2 beam line at BESSYII in Berlin. The resonant photoemission spectra (resPES) at the carbon K-edge give a complete picture of the occupied and unoccupied states in these sp² hybridized system. Above the K-edge the resPES data are dominated by the Auger process causing a C2p4 final state. The Auger lines appear at constant kinetic energy (spectator, 2h) or constant binding energy (participator, 1h). For the features right at the resonance we observe a different Auger decay mechanism. We attribute it to the decay out of an excitonic intermediate state with a long lifetime. It involves three valence hole states. The original primary core hole is filled by a normal KLL Auger decay. The excited electron rests in the excitonic intermediate state and decays later. We discuss the spectral features of such combined spectator-participator decays in detail which are found only close to resonance and only in the localized valence states of excitonic excitation i.e. C1s - 1 π^* transitions [1, 2, 3]. [1] Richter et al. (2011) BioNanoScience, submitted. [2] Michling et al. (2011) IOP C Ser Mater Sci Eng, submitted. [3] Schmidt et al. (2011) Solid State Ionics, submitted.

DS 35.5 Thu 18:45 H 2032

Nanoscale assembly, morphology and screening effects in nanorods of newly synthesized substituted pentacenes

— •MARIA BENEDETTA CASU¹, SABINE-ANTONIA SAVU¹, SIMON SCHUNDELMEIER¹, SABINE ABB¹, CHRISTINA TÖNSHOFF², HOLGER F. BETTINGER², and THOMAS CHASSÉ¹ — ¹Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany — ²Institute of Organic Chemistry, University of Tübingen, Tübingen, Germany

We have investigated nanorods of two newly synthesized substituted pentacenes deposited on Au(111): δ 4-substituted (2,3-X2-9,10-Y2) pentacene with X = Y = methoxy group and X = Fluorine, Y = methoxy, by using X-ray photoemission spectroscopy (XPS) and atomic force microscopy (AFM). Energy dependent photoemission spectra show complex features that we have analyzed in detail by using a fitting procedure. Our analysis reveals the unusual presence of surface core level shifts due to the high electronegativity of the fluorine atoms and the structure of the nanorods. In addition, the distinctive features of growth and morphology of the nanorods are subjected to a template effect by the substrate lattice geometry, leading to a systematic organization of the nanorod assemblies.

DS 35.6 Thu 19:00 H 2032

Organic Field-Effect Transistor Operation With Different Gatings — •NIS HAUKE HANSEN¹, CARINA WUNDERLICH¹, and JENS PFLAUM^{1,2} — ¹Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — ²ZAE Bayern e.V., D-97074 Würzburg

To enable superior insulation characteristics together with low-voltage operation, e.g. for portable electronic devices, organic thin film transistors (TFT) can be gated by ultrathin self-assembled monolayer (SAM) dielectrics [1]. Alternatively, the choice of ionic liquids (IL) as gate dielectric allows for accumulation of high charge carrier densities in the order of 10¹³ cm⁻², corresponding to a charge carrier doping of up to 0.3 holes per molecule. In this contribution we employed both approaches to gate TFTs based on vacuum sublimed Pentacene (PEN) and Diindenoperylene (DIP) films as semiconducting channel. The observed current-voltage (IV) characteristics show low threshold voltages between -3 and -1 V for all devices under investigation and hole mobilities up to 10⁻¹ $\frac{\text{cm}^2}{\text{Vs}}$ for SAM gate dielectrics in combination with

PEN as well as DIP. Utilizing an IL as gate dielectric high charge carrier densities in the order of 10^{13} cm^{-2} have been confirmed. In order to correlate the electronic performance with thin film morphology, atomic force microscopy (AFM) and x-ray diffraction (XRD) measurements have been performed indicating the influence of the respective gating on the structural properties of the molecular semiconductors.

[1] H. Klauk, et al., Nature 445 (2007) 745

DS 35.7 Thu 19:15 H 2032

A comparative study of the absorption spectra of binary mixtures of organic semiconductors — •KATHARINA BROCH¹, AN-TJE AUFDERHEIDE¹, JENS REINHARDT¹, ALEXANDER HINDERHOFFER¹, CHRISTIAN FRANK¹, FALK ANGER¹, REINHARD SCHOLZ², ALEXANDER GERLACH¹, and FRANK SCHREIBER¹ — ¹Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — ²Technische Universität Dresden, Institut für Angewandte Photo-

physik, George-Bähr-Straße 1, 01069 Dresden

Mixtures of organic semiconductors can be used to increase the donor-acceptor interface in organic optoelectronic devices. However, the influence of molecular geometry and chemical structure on the mixing behaviour as well as on the optical properties is still not completely understood. We present a comparative study of binary mixtures of three organic semiconductors, i.e. pentacene (PEN), perfluoropentacene (PFP) and diindenoperylene (DIP), in different combinations [1,2]. Using spectroscopic ellipsometry we study the optical properties of the mixed films including possible intermolecular interactions. By comparing the spectroscopic results with detailed x-ray data [3,4], we discuss the influence of the mixing behaviour and structural properties on the absorption spectra of the intermixed films.

[1] K. Broch et al., Phys. Rev B, **83**, 245307 (2011). [2] J. P. Reinhardt et al., in preparation [3] A. Hinderhofer et al., J. Chem. Phys., **134**, 104702 (2011). [4] A. Aufderheide et al., in preparation