

## DS 64: Organic Thin Films III

Time: Friday 14:00–15:45

Location: GER 38

DS 64.1 Fri 14:00 GER 38

**Alkali metal-intercalated Picene thin films: Examination of the electronic structure by photoemission spectroscopy** —

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Recently, superconductivity was reported for potassium-doped picene single crystals (K<sub>3</sub>Pic) from magnetization measurements [1]. We have investigated A<sub>x</sub>Pic thin films (A=K, Cs) on silicon oxide substrates by means of photoemission spectroscopy (PES) to follow the evolution of the spectral function with doping. The high quality of our Pic films is demonstrated by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). To clarify the growth mode of the films, surface images were taken with an atomic force microscope (AFM). In the PES spectra one can observe the gradual filling of the former lowest unoccupied molecular orbital (LUMO) with alkali metal evaporation time. As opposed to previous experiments on K-doped pentacene films, a two-peak structure, instead of one, appears in the former gap of the organic semiconductor. The origin of these features has not been unraveled as yet. We discuss these findings as well as the absence of a clear metallic Fermi cut-off against the background of experimental and theoretical work so far.

[1] R. Mitsuhashi *et al.*, Nature **464**, 76 (2010)

DS 64.2 Fri 14:15 GER 38

**Interaction between Cobalt Phthalocyanine and Gold Revealed by Photoexcited Electron Spectroscopies** —

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Cobalt phthalocyanine (CoPc) monolayer films evaporated on Au(100) are studied by photoexcited electron spectroscopies (XPS, XAES, UPS, XAS, ResPES). A quite intense modification of the electronic structure of the CoPc molecule at the interface with Au, with respect to the molecule in the bulk phase, is observed by XPS, UPS and XAES (X-ray excited Auger electron spectroscopy). Local charge transfer towards the central metal atom of the phthalocyanine molecule from the gold substrate affects the charge state of the Co ion resulting in a different line shape of the Co related peaks and the presence of enhanced features in the energy region across the metal d-bands (UPS). This could be explained by a mixing of the transition metal 3d states with the underlying metallic states of gold. This suggestion is further supported by XAS data according to which, the Co 2p absorption spectra look different for monolayer and thicker organic films pointing to a possible interaction of the molecules with the substrate via the Co d-electrons. Co-related valence band states of CoPc were identified by Resonant Photoemission (ResPES).

DS 64.3 Fri 14:30 GER 38

**Electronic structure and optical properties of P3HT - Evidence of 2D-polarons in P3HT** —

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In this contribution we report on investigations of the electronic structure and optical characteristics of poly(3-hexylthiophene) (P3HT) based films. Various techniques like NEXAFS, SRXPS, UPS, UV-VIS and FTIR were used. X-Ray based measurements were done at the U49/2-PGM2 beam line at BESSYII. The samples were produced by spin casting P3HT dissolved in chloroform and other suitable solvents on ITO (indium tin oxide) coated glass slides and silicon substrates. Regioregular-P3HT is known to form thin films with nanocrystalline lamellae. This 2D structure give rise to additional electronic excitations in photoinduced absorption measurements, which are attributed to 2D-polarons [1]. In the Total Electron Yield (surface sensitive) and Total Fluorescence Yield (bulk sensitive) NEXAFS spectra of regioregular-P3HT three additional features can be found prior to the

first typical  $\pi^*$  excitation. The nature of these features was further investigated by means of SRXPS and UPS measurements. Energy differences relative to  $\pi^*$ -peak maximum (0.54eV, 0.87eV and 2.24eV) suggest that these features are due to 2D-polarons. This presence of polarons is further confirmed by our FTIR and UV-VIS results. [1] Osterbacka *et al.*, Synth. Met. **116** (2001) 317

DS 64.4 Fri 14:45 GER 38

**Correlation between the interface-energetics and thermal stability of SAMs on Gold** —

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Improved organic electronic device characteristics can be achieved via SAM-modification, which is attributed to enhanced crystal growth and a lowering of the injection barrier. A variety of thiol-based SAMs was used for an UPS-study to elucidate structure-related properties in such systems. We could generalize the dependency of the workfunction change on the alkanethiol-SAM dipoles to more complex systems based on functionalized aromatic backbones. By adjusting the size of a given SAM or substituting atoms the molecular dipole and subsequently the interface dipole can be tuned.

In addition we employed thermal desorption spectroscopy to correlate the magnitude of the covalent interactions between the SAM's sulfur groups and the gold to the interface energetics. We have indications that, for the investigated systems, varying the SAM functionalization does not affect the sulfur-gold-bonding, which is in close agreement to the findings of Heimel *et al.* in 2008, reporting that the thiol- and the headgroup of a particular SAM are electronically decoupled.

DS 64.5 Fri 15:00 GER 38

**Investigation of electronic properties and morphology of an n-channel perylene tetracarboxylic diimide thin film** —

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We report on the influence of thickness and substrate on the electronic density of states and on the surface potential of an air-stable n-channel perylene tetracarboxylic diimide semiconductor thin film. Ultra-violet photoelectron spectroscopy (UPS) and Inverse photoelectron spectroscopy (IPES) show a variation of the band gap and of the electron affinity of the material as a function of substrate. The organic thin films were fabricated with Polyera ActivInk™ N1200 (PDI8-CN<sub>2</sub>) by molecular beam deposition on Gold or native Siliconoxide and then analyzed in an ultra-high vacuum chamber without exposure to ambient atmosphere.

The thin films were further investigated under ambient conditions using an atomic force microscope (AFM) to gain information of the topography. Additional Kelvin-Probe force microscopic (KPFM) measurements give insight into the local resolved surface potential.

DS 64.6 Fri 15:15 GER 38

**UV-induced sample degradation can mimic band bending during photoemission of organic thin films** —

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Photoemission spectroscopy (PES) has evolved to a widely used method for characterizing conjugated organic materials' electronic structure at interfaces. Noteworthy, energy level shifts ascribed to band bending in thickness-dependent studies of organic thin films are often not unequivocally reproducible. We show for prototypical thiophene-based molecular and polymer materials that such energy shifts may in fact be induced by the PES measurement itself. The valence spectra of thin films on PEDT:PSS and Au exhibit irreversibly rigid shifts by up to 0.4 eV to higher binding energies, without notable changes of the spectral shape. This shift is a monotonous function of

ultraviolet (UV) light irradiation time and photon flux. Photo-electron induced defects may be created in the sample that either lead to gap states, which shift the Fermi-level, or to the build-up of space charges. The degradation proceeds at a lower rate if a high-conductivity substrate is used for the organic materials, indicating that photo-electron induced degradation is enhanced by subtle sample charging.

DS 64.7 Fri 15:30 GER 38

**Imaging ellipsometry of graphene** — •PETER H. THIESEN<sup>1</sup>, CHRISTIAN RÖLING<sup>1</sup>, and ULRICH WURSTBAUER<sup>2</sup> — <sup>1</sup>Accurion GmbH, Stresemannstr. 30, 37079 Göttingen — <sup>2</sup>Physics Department, Columbia University, New York, NY 10027

A graphene monolayer flake on a SiO<sub>2</sub> (300 nm)|Si substrate was characterized. The sample was previously imaged by optical and atomic force microscopy and identified as a graphene monolayer by RA-

MAN spectroscopy. Ellipsometric contrast micrographs were recorded. Wavelength spectra of Delta and Psi at different angles of incidence were measured, as well as creation of Delta and Psi-maps. As described in literature, the determination of the dispersion function of graphene is done under the assumption of a layer thickness of 0.35 nm but using a Drude oscillator model. The spectra of Delta and Psi of the Graphene crystallites are significantly different from the substrate and the surrounding graphite flakes. The Dispersion function is in good agreement with literature values when using the same layer thicknesses.

Imaging ellipsometry offers the opportunity to measure the optical properties of graphene flakes at sizes typical for micro-mechanical cleavage. Ellipsometric contrast micrographs, in combination with Psi-maps, are promising tools for locating and identifying graphene crystallites. This was shown for the classic SiO<sub>2</sub>|Si substrate as well as for GaAs.