DS 48: [O] Organic Electronics and Photovoltaics III (Joint Session DS/CPP/HL/O)

Time: Friday 11:15–12:45 Location: H40

DS 48.1 Fri 11:15 H40

WO3 under, in and on CuPc - A doping mechanism for organic semiconductors — •Corinna Hein, Eric Mankel, Thomas Mayer, and Wolfram Jaegermann — TU Darmstadt, FG Oberflächenforschung, Petersenstraße 32, 64287 Darmstadt

Doping of organic semiconductors plays an important role for the development of organic devices like photovoltaic cells or organic light emitting diodes. P-doping of CuPc which is frequently used as hole conductor was performed successfully by coevaporation of the CuPc matrix and the WO3 dopant showing good doping efficiency and limit. The Fermi level determined by synchrotron induced photoemission shifts gradually with the concentration of dopant up to 690meV. To clarify the doping mechanism band alignment of both CuPc/WO3 and WO3/CuPc interfaces was determined. The work function difference of the two materials is overcome by band bending and an interface dipole. The dipole is 2eV for CuPc/WO3 and 1.4eV for WO3/CuPc lowering the amount of transferred charge and therefore limiting the doping efficiency. The sum of band bending at the interface adds up to 0.5eV for the CuPc/WO3 interface and 1.1eV for CuPc deposited on WO3. The Fermi level shift in the composites fits to this range in accord to a doping model assuming cluster growth of WO3 within CuPc. The model could be directly proofed by transmission electron microscopy distinguishing the two phases of CuPc and WO3 with a cluster size of approximately 5nm.

DS 48.2 Fri 11:30 H40

Mixed Self-Assembled Monolayers on Au(111): Understanding the Level Alignment and Work-Function Modification. — •Ferdinand Rissner[1], David A. Egger[1], Lorenz Romaner[2], Georg Heimel[3], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria — [3]Institut für Physik, Humboldt-Universität zu Berlin, Germany

In organic electronics, coverage of electrodes with appropriate self-assembled monolayers (SAMs) is a well-known technique for enhancing the performance of devices; by modification of the electrode work function, Φ, charge-carrier injection barriers can be optimized. Mixing molecules which show a work-function increasing effect $(\Delta\Phi > 0)$ with molecules decreasing Φ was experimentally found to allow for tuning of Φ over a wide range (as a function of the mixing ratio). [1]

For "pure" SAMs of π-conjugated oligophenylene derivatives, the mechanisms controlling the metal/SAM interface energetics have been extensively investigated over the past years. Here, we present density-functional theory based slab-type band structure calculations on the energetics of mixed monolayers. We find and explain significant differences in the energy-level alignment compared to what is known from the respective pure layers.

[1] K.-Y. Wu, S.-Y. Yu and Y.-T. Tao, Langmuir, **2009**, 25 (11), pp 6232-6238.

DS 48.3 Fri 11:45 H40

Analysis of systematic heat treatment of TiO2 nanocrystalline films for solid-state dye sensitized solar cells using photoelectron spectroscopy — •Xianjin Feng, René Hock, Eric Mankel, Thomas Mayer, and Wolfram Jaegermann — Institute of Materials Science, Darmstadt UniVersity of Technology, D-64287 Darmstadt, Germany

In this contribution we investigated the effect of heat treatment on the chemical and electronic structures of TiO2 nanocrystalline films for solid-state dye sensitized solar cells (SDSC). The samples were heated in air by an air-gun and a hot plate, respectively, within the temperature range of 300-600°C. The samples were chemically and electronically characterized using synchrotron-induced photoelectron spectroscopy (SXPS) and X-ray photoemission spectroscopy (XPS). The most prominent chemical variation after heating by air-gun was found in the SXPS the intensity increase of the Na2p core level and obvious changes both in the O2s core level and O2p valence band were also observed at 450°C. An increase in the Na1s core level was also observed in the XPS study. For the heat treatment using a hot plate, the intensity of the Na2p core level increased less strongly and no obvious change in the O2s core level and O2p valence band was observed even at 600°C. In both cases of heat treatment, the oxygen vacancies VO-related gap states around 1.3 eV and states just below the Fermi level were observed in the gap region and the intensity of the VO-related gap states decreased obviously after heating and almost vanished at high temperatures.

DS 48.4 Fri 12:00 H40

Vanadyle and perfluoro vanadyle phthalocyanine on gold: unseen metastable modification and interfacial reaction — •Indro Biswas, Heiko Peisert, and Thomas Chassé — Institut f. Physikalische u. Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, 72076 Tübingen

Vanadyle phthalocyanine (PcVO) and perfluorinated-vanadyle phthalocyanine (F_{16}PcVO) are of the same inside-out-umbrella structure as the extensively investigated titanyle phthalocyanine. Just in the recent years, interest on these molecules has grown again. They exhibit some very surprising properties. Thin films of PcVO and F_{16}PcVO on polycrystalline gold have been examined using photoemission, X-ray absorption, optical spectroscopy, and Kelvin probe measurements. In addition to surprisingly good self-ordering abilities of both materials, an interface reaction including the fluorine substituents in F_{16}PcVO has been observed, and the application of the minimal invasive Kelvin probe method allowed the investigation of the undisturbed metastable Phase I of PcVO with a different interface formation, which will be transformed by conventional spectroscopic methods.

1 C. H. Griffiths, M. S. Walker, P. Goldstein, *Polymorphism in Vanadyle Phthalocyanine*, Mol. Cryst. Liq. Cryst. 33 (1976) 149.

DS 48.5 Fri 12:15 H40

Photoemission spectroscopy investigations of silicon organic dye interfaces for photovoltaic applications — •Andreas Decker[1], Thomas Mayer[1], Wolfram Jaegermann[1], Sabin Suraru[2], and Frank Würthner[2] — [1]Fachgebiet Oberflächenforschung, Fachbereich Materialwissenschaften, Technische Universität Darmstadt — [2]Institut für Organische Chemie, Universität Würzburg

In a new solar cell concept, organic dyes (small molecules) are embedded in the hydrogenated microcrystalline i-layer of a silicon p-i-n structure to enhance the optical absorption. This approach aims at an increase in efficiency and a decreased silicon absorber layer thickness, thus potentially lowering deposition time and production cost.

The electrical lineup of the dye orbitals versus the silicon band edges plays a vital role for this sensitization process because a driving force is needed for the transfer of photogenerated electrons and holes from the dye molecules to the silicon matrix. For the two dyes Cl$_4$MePTCDI and CuPc the electrical lineup on our model substrate, hydrogen terminated n-type Si(111), was investigated with photoemission interface experiments. Si(111):H was prepared from wafers with a native oxide by two-step wet-chemical etching in NH$_4$F which leads to clean and flat terraces as shown in AFM measurements. By comparison of calculations with XPS measurements the Si(111):H surface was found to have flat bands, i. e. showing no Fermi level pinning due to dangling bonds or fresh adsorbates originating from the sample transport through air to the UHV system, thus being a suitable substrate for interface experiments.

DS 48.6 Fri 12:30 H40

Band alignment studies of ZnO-ZnS-CIS interfaces — •Carsten Lehmann, Andreas Hofmann, Alexandra Dombrowa, and Christian Pettenkofer — Helmholz-Zentrum Berlin, Berlin, Deutschland

With respect to thin film solar cells based on CuInS$_2$ and ZnO ZnS is a promising alternative to CdS as buffer layer material [1,2]. A MOMBE process based on diethylzinc and water is investigated on CuInS$_2$(112) thin films. A ZnS buffer layer grows epitaxially using the surplus of sulfur in the eventually present CuS$_x$ layer. A ZnO film grows on top of the .8 nm thick ZnS layer with its own lattice parameters in (0001) direction. Step-by-step analysis of this ZnO-ZnS-CIS interface yielded a band alignment favorable for photovoltaic applications [2]. We present in-situ preparation and step-by-step investigation on ZnO-ZnS-CIS interfaces with varying CIS substrates. CuInS$_2$(001) samples were prepared on GaAs(100) by gas source MBE (GSMBE) using TBDS as sulfur precursor. Sulfurization of CuIn films prepared by MBE and sputtering yielded polycrystalline CuInS$_2$ samples of 100nm up to 2.5μm thickness. The samples were investigated by XPS, UPS and LEED. We will discuss the interfaces with respect to the derived band aligments and their morphology. Furthermore we will compare the results to those of analogous experiments on $CuInSe_2$(112). [1] M. Bär, et. al., Journal of Applied Physics 99 (2006) [2] S. Andres, et. al., Thin Solid Films 518 (2009)