

CPP 64: Organic-Inorganic Hybride Interfaces (joint session CPP/DS/HL, organized by DS)

Time: Friday 9:30–11:45

Location: CHE 91

CPP 64.1 Fri 9:30 CHE 91

Hybrid organic-inorganic nano-structures studied by HR-PES and HR-TEM — ●OLGA MOLODTSOVA^{1,2}, SERGEY BABENKOV¹, IRINA ARISTOVA³, ANDREI HLOSKOVSKY¹, DENIS VYALIKH⁴, DMITRY SMIRNOV⁵, KARINA SCHULTE⁶, and VICTOR ARISTOV^{1,3,7} — ¹DESY, Hamburg, Germany — ²ITMO, Saint Petersburg, Russia — ³ISSP RAS, Chernogolovka, Russia — ⁴TU Dresden, Germany — ⁵BESSY, Berlin, Germany — ⁶Max-lab, Lund, Sweden — ⁷TU Bergakademie, Freiberg, Germany

Morphology and the electronic properties of hybrid organic-inorganic systems, composed of metallic nanoparticles which are self-organized in organic semiconductor thin film of phthalocyanines complexes were studied by transmission electron microscopy and photoelectron spectroscopy using synchrotron radiation.

CPP 64.2 Fri 9:45 CHE 91

STM and PES Investigations of Organic-TMD Heterointerfaces: Self-Assembly and Energy Level Alignment — ●THORSTEN SCHULTZ¹, YULI HUANG^{2,3}, ZHIBO SONG^{2,3}, ZIJING DING², LAIN-JONG LI⁴, DONGZHI CHI², PATRICK AMSALEM¹, ANDREW WEE³, and NORBERT KOCH¹ — ¹Humboldt-Universität zu Berlin, Germany — ²Agency for Science, Technology and Research, Singapore — ³National University of Singapore — ⁴King Abdullah University of Science and Technology, Saudi Arabia

The growing interest in two-dimensional transition metal dichalcogenide (TMD) materials brings additional opportunities for interfacing with organic molecules to fabricate flexible organic/inorganic devices. However, the complex interfacial properties at the organic-TMD heterointerfaces, including the growth behavior and energy level alignment (ELA) that determine the device performance, are still not well understood. Combining scanning tunneling microscopy/spectroscopy (STM/STS) with photoemission spectroscopy (PES), we are able to probe the self-assembly of fluorinated fullerene C60F48 on single-layer WSe2 deposited on a graphite substrate and its interfacial electronic properties. From our studies it is found that the interfacial dipole together with charge transfer play critical roles in determining the phase evolution of the C60F48 molecules adsorbed on the surface, as well as the ELA at the C60F48/WSe2/graphite heterointerface.

CPP 64.3 Fri 10:00 CHE 91

Energy Level Control at ZnO/Organic Semiconductor Interfaces — ●RAPHAEL SCHLESINGER¹, SYLKE BLUMSTENGEL¹, STEFANIE WINKLER², JOHANNES FRISCH¹, JENS NIEDERHAUSEN¹, RUSLAN OVSYANNIKOV², ANTJE VOLLMER², FRITZ HENNEBERGER¹, and NORBERT KOCH^{1,2} — ¹Humboldt-Universität zu Berlin, Institut für Physik — ²Helmholtz-Zentrum Berlin - BESSY II

Hybrid inorganic organic systems (HIOS) are promising candidates for future (opto-)electronic devices by taking advantage of the complementary beneficial properties of two different material classes. However, inadequate interfacial energy level alignment is an intrinsic obstacle to superior device function. Hence, to design efficient HIOS devices, understanding and controlling HIOS energy level alignment is a key factor.

In this contribution we employ molecular electron donor or acceptor interlayers to tune the work function (ϕ) of ZnO between 2.2 eV (by using the organometallic donor [RuCp*mes]₂) and 6.4 eV (by using F4TCNQ). Only for molecular acceptor adsorption, significant adsorption induced upward band bending of up to 0.9 eV is found within ZnO. Exploiting the huge ϕ modifications of ZnO, up- and downward HIOS energy level readjustments are shown, which realize ultimately low electron- or hole-injection barriers. Moreover, by using an OSC whose gap matches that of ZnO, the energy level offsets at the HIOS interface could be eliminated. This enables highly efficient, non-quenched energy transfer across the HIOS interface, which is usually inhibited by unfavorable energy level alignment.

CPP 64.4 Fri 10:15 CHE 91

Structure of van der Waals bound Hybrids of Organic Semiconductors and Transition Metal Dichalcogenides: the Case of Acene Films on MoS2 — ●TOBIAS BREUER, TOBIAS MASSMEYER, ALEXANDER MÄNZ, STEFFEN ZOERB, BERND HARBRECHT, and GREGOR WITTE — Philipps-Universität Marburg, Ger-

many

Transition metal dichalcogenides (TMDC) are important representatives in the emerging field of two-dimensional materials. At present, their combination with molecular films is discussed as it enables the realization of van der Waals bound organic/inorganic hybrids which are of interest in future device architectures. Here, we discuss the potential use of molybdenum disulfide (MoS₂) as supporting substrate for the growth of well-defined, crystalline organic adlayers. By this means, hybrid systems between the TMDC surface and organic compounds can be prepared, allowing for the profound investigation of mutual optical and electronic coupling mechanisms. As model system, we choose pentacene and perfluoropentacene as prototypical organic semiconductors and analyze their film formation on MoS₂(001) surfaces. In both cases, we observe smooth, crystalline film growth in lying molecular configuration, hence enabling the preparation of welldefined hybrid systems. By contrast, on defective MoS₂ surfaces both materials adopt an upright molecular orientation and exhibit distinctly different film morphologies. This emphasizes the importance of highly ordered TMDC surfaces with low defect density for the fabrication of well-defined hybrid systems.

[1] T. Breuer et al., PSS RRL (2016), DOI: 10.1002/pssr.201600320

15 min. break.

CPP 64.5 Fri 10:45 CHE 91

Real-Time Investigation during Au sputter deposition on polymer and SiOx surfaces. — ●MATTHIAS SCHWARTZKOPF¹, ANDRÉ ROTHKIRCH¹, BJÖRN BEYERSDORFF¹, CALVIN BRETT¹, MARC GENSCHE¹, WIEBKE OHM¹, OLEKSANDR POLONSKYI², ALEXANDER HINZ², THOMAS STRUNSKUS², ADRIAN HAUSMANN³, FRANZISKA LÖHRER³, VOLKER KÖRSTGENS³, FRANZ FAUPEL², PETER MÜLLER-BUSCHBAUM³, and STEPHAN ROTH^{1,4} — ¹DESY, Notkestr. 85, D-22607 Hamburg — ²CAU zu Kiel, Kaiserstr.2, D-24143 Kiel — ³TUM, James-Frank-Str. 1, D-85748 Garching — ⁴KTH, Teknikringen 56-58, SE-100 44 Stockholm

The reproducible low-cost fabrication of functional polymer-metal nanocomposites remains a major issue in applied nanotechnology. In order to obtain full control over the nanostructural evolution at the metal-polymer interface, we employed the combination of time-resolved surface sensitive X-ray scattering with optical measurements during sputter deposition of gold on thin polystyrene films [1] and SiOx [2]. We correlate the evolution of the metallic layer morphology with changes in the key scattering features. This enabled us to identify the impact of substrate effects on the growth regimes with their specific thresholds and their resulting optical properties. Our study opens up the opportunity to improve nanofabrication of tailored metal-polymer nanostructures for organic electronics like photovoltaic applications and plasmonic-based technologies. [1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015); [2] Schwartzkopf et al., Nanoscale 5, 5053 (2013).

CPP 64.6 Fri 11:00 CHE 91

Analytical Study of Solution-Processed Nickel Oxide and its Application in Organic Electronics - (1) Photoelectron Spectroscopy — ●FLORIAN ULLRICH^{1,4}, VALENTINA ROHNACHER^{2,4}, JAKOB BOMBSCH^{3,4}, WOLFRAM JAEGERMANN^{1,4}, and ERIC MANKEL^{1,4} — ¹TU Darmstadt, Materials Science Institute — ²University of Heidelberg — ³TU Braunschweig — ⁴InnovationLab

For the fabrication of efficient organic solar cells (OPV) suitable extraction layers are needed. A material fulfilling the requirements and leading to superior efficiencies in comparison to the standard material PEDOT:PSS is nickel oxide (NiO).

In this work we want to contribute to a more detailed understanding of the relations between annealing temperature of solution-processed NiO (sNiO), surface treatments, bulk and surface composition, structure and properties, ability to form self-assembled monolayers (SAMs) and the characteristics of sNiO-based OPV. For that purpose different analytical methods like x-ray photoelectron spectroscopy (XPS) and infrared spectroscopy (IR) were conducted and various OPVs were built and characterized.

In this first part we use XPS to monitor changes of band bending and surface dipoles induced by surface treatments like oxygen plasma (OP)

or deposition of SAMs. These information help to explain characteristics of corresponding OPVs and provide valuable hints for the design of more efficient devices. We show how band alignment can controllably be improved by adjusting the work function via varying annealing temperature of sNiO films, OP treatment and SAM molecules.

CPP 64.7 Fri 11:15 CHE 91

Analytical study of Solution-processed Nickel Oxide and its Application in Organic Electronics: (2) Infrared Spectroscopy — ●VALENTINA ROHNACHER^{1,2}, SABINA HILLEBRANDT^{1,2}, FLORIAN ULLRICH^{2,3}, JAKOB BOMBSCH^{2,4}, SEBASTIAN BECK^{1,2}, and ANNEMARIE PUCCI^{1,2} — ¹Kirchhoff-Institut für Physik, Universität Heidelberg — ²InnovationLab, Heidelberg — ³TU Darmstadt — ⁴TU Braunschweig

The performance of organic photovoltaic cells (OPVs) is significantly influenced by the properties of the interfaces between the layers. Increasing the interfacial compatibility especially between the transparent conductive oxide electrode and the organic semiconductor layer can improve the charge carrier transport through the stack and thus the efficiency of the device. Thin films of nickel oxide (NiO) have shown promising characteristics as hole extraction layers in OPVs. In our studies, solution-processed NiO surfaces were passivated by self-assembled monolayers (SAMs) to tune the work function and to reduce the surface reactivity. Infrared spectroscopy gives insight into the composition of the investigated material and can monitor orientation of characteristic vibrations or functional groups. The results show that temperature and plasma treatment dramatically change the surface properties and that especially nickel hydroxide and nickel oxyhydroxide play an important role for the binding mechanism of SAMs.

Together with photoelectron spectroscopy and OPV device characteristics a better understanding of the energetic and chemical properties at the interface was achieved helping to improve device performance.

CPP 64.8 Fri 11:30 CHE 91

Analytical Study of Solution-Processed Nickel Oxide and its Application in Organic Electronics: (3) Application in Organic Solar Cells — ●JAKOB BOMBSCH^{1,2,4}, SEBASTIAN HIETZSCHOLD^{1,2,4}, VALENTINA ROHNACHER^{2,4}, FLORIAN ULLRICH^{3,4}, ROBERT LOVRINCIC^{1,4}, and WOLFGANG KOWALSKY^{1,2,4} — ¹TU Braunschweig — ²Uni Heidelberg — ³TU Darmstadt — ⁴InnovationLab, Heidelberg

Nickel oxide (NiO) has shown promising properties as a carrier-selective hole contact material with high transparency, and a good matching ionization potential to most donor materials [1,2]. Here we apply solution-processed NiO films as an interlayer in small molecule flat- and bulk-heterojunction solar cells with F4ZnPc and C60 as a donor and acceptor, respectively, and correlate the observed IV-characteristics with annealing temperature, thickness, and surface post-treatment of the NiO layer. While oxygen plasma treatment improves device performance, the application of dipolar self-assembled monolayers lead to strongly S-shaped IV curves. To examine the nature of the barrier introduced, we vary the doping density of the NiO film by adding copper oxide. Together with data from Infrared spectroscopy and Photoelectron spectroscopy measurements, we gain a more fundamental understanding of the impact of NiO surface properties on solar cell performance. [1] Manders, J. R. Et al. *Adv. Funct. Mater.*, 23: 2993-3001 (2013). [2] Schulz, P. et al. *Adv. Funct. Mater.* 24, 701-706 (2014).