

CPP 58: Organic Thin Films, Organic-Inorganic Interfaces: Session I (joint session DS/CPP)

Time: Wednesday 16:00–18:15

Location: H 0111

Invited Talk

CPP 58.1 Wed 16:00 H 0111

Prospects of Engineering Chemistry and Electronic Character of Interfaces in Multifunctional (Bio)Organic-Inorganic Hybrids — ●MARIA LOSURDO — Institute of Nanotechnology, CNR-NANOTEC, Bari, Italy

New opportunities for energy harvesting, plasmonics, active photonics, biomimetic catalysis, biosensing, immunosensing and cellular recognition are offered by novel hybrid heterojunctions combining, semiconductors, plasmonic metal nanostructures and (bio)-organic systems.

In order to design these (bio)-organic/inorganic platforms, the establishment of reliable and reproducible protocols for their functionalization is still needed, which require better understanding of the surface and interfacial electronic phenomena.

This contribution presents strategies for tailoring the chemistry and electronic character of interfaces in hybrids spanning from planar surfaces (semiconductors Si, III-Vs, TCOs, SiC) to nanosystems (plasmonic Au, Ga, Al) designed to enable applications in photovoltaics (hole transport organic layers and semiconducting new polymers), biomimetic catalysis (porphyrins) and bio-immuno-sensing (proteins, DNA, cells).

The emphasis will be on functionalization methods, including plasma treatments of surfaces and interfaces, resulting assembly and nanostructures and how the interface chemistry determines the charge transfer enabling the specific functionality.

Future directions towards the rational design of those hybrids will be suggested.

15 min. break.

CPP 58.2 Wed 16:45 H 0111

Synthesis and combined experimental and theoretical characterization of dihydro-tetraaza-acenes — ●BERND KOLLMANN¹, ZHONGRUI CHEN², DANIEL LÜFTNER¹, OLIVIER SIRI², and PETER PUSCHNIG¹ — ¹Institute of Physics, University of Graz, NAWI-Graz, Universitätsplatz 5, 8010 Graz, Austria — ²Aix Marseille Université, CNRS, CINaM UMR 7325, 13288 Marseille, France

We present a combined experimental and theoretical study of electronic and optical properties of dihydro-tetraaza-acenes (DHTAn). Using a solvent-free condensation, we are able to synthesize DHTA5, DHTA6 and DHTA7 molecules. We investigate their gas-phase electronic structures of by means ab-initio density functional calculations employing an optimally-tuned range-separated hybrid functional. By comparing with the parent linear oligoacenes (nA) and based on computed ionization potentials and electron affinities, we predict DHTAn molecules to be more stable than acenes of the same length, where we expect DHTAn molecules to be persistent at least up to $n = 7$ rings. We further exploit the analogy with nA by analyzing the entire intramolecular π -band structure of the DHTAn molecules. This clearly reveals that the additional two electrons donated by the dihydropyrazine group are delocalized over the entire molecule and contribute to its π -electron system. As a consequence, the symmetry of the frontier orbitals of DHTAn differs from that of the parent nA molecule. This is also illustrated by the UV-vis absorption spectra which have been measured for DHTA5, 6 and 7 dissolved in dimethyl sulfoxide and analysed by means of excited state calculations with an time-dependent DFT framework.

CPP 58.3 Wed 17:00 H 0111

photochromic phosphonic-acid diarylethene self-assembled monolayer switches on polar ZnO surfaces — ●QIANKUN WANG¹, GIOVANNI LIGORIO¹, VALENTIN DIEZ-CABANES², DAVID CORNIL², BJÖRN KOBIN³, STEFAN HECHT³, JÉRÔME CONIL², EMIL J.W. LIST-KRATOCHVIL¹, and NORBERT KOCH¹ — ¹Institut für Physik, Humboldt-Universität zu Berlin — ²Laboratory for Chemistry of Novel Materials, University of Mons — ³Department of Chemistry, Humboldt-Universität zu Berlin

Here, we investigate the interfacial chemical and switching properties of the phosphonic-acid diarylethene (PA-DAE) switch in form of a self-assembled monolayer (SAM) on ZnO(0001) and ZnO(000-1) surfaces by photoelectron spectroscopy and density functional theory calculations. The observed work function increase is attributed to the introduction of a surface dipole; the binding modes of the phosphonic-acid linker were retrieved from the deconvolution of O 1s core level

spectra, indicating the formation of mixed bidentate and tridentate binding. The quantification of core level spectra supports the picture of a densely packed SAM on both ZnO surfaces. Upon illumination with ultraviolet and visible light, respectively, we observe a 0.7 eV energy level shift at the onset of the highest occupied molecular orbital (HOMO) level of the PA-DAE molecules. This can further on be used to reversibly switch the energy level alignment at the ZnO/PA-DAE interface in device structures.

CPP 58.4 Wed 17:15 H 0111

Investigation of sputter deposited nanostructured alloy films on polymer surfaces — NIKO CARSTENS¹, ALEXANDER HINZ¹, OLEKSANDR POLONSKYI¹, ●THOMAS STRUNSKUS¹, MATTHIAS SCHWARTZKOPF², PALLAVI PANDIT², ANDRE ROTHKIRCH², FRANZISKA LÖHRER³, VOLKER KÖRSTGENS³, SIMON SCHAPER³, PETER MÜLLER-BUSCHBAUM³, STEPHAN ROTH², and FRANZ FAUPEL¹ — ¹Chair for Multicomponent Materials, CAU Kiel, 24143 Kiel — ²DESY, 22607 Hamburg — ³Physcis Department, TU Munich, 85748 Garching

The fabrication of functional materials with tailored plasmonic properties gained much interest in recent years. Vapor phase deposition techniques like sputtering are an attractive approach to produce self-assembled nanostructured films which exhibit plasmonic activity when the effective thickness is under the percolation threshold. As the local surface plasmon resonance can be tuned by the composition, alloy films are of special interest. In this study, the growth of miscible (AuAg) and immiscible (CuAg) systems on different polymer surfaces (PS and PMMA) by magnetron sputtering has been investigated. The correlation between optical properties and the stage of film growth was examined during deposition by means of in-situ reflection UV-Vis spectroscopy as well as time resolved GIWAXS and GISAXS investigations [1,2]. In addition, SEM investigations as well as ex-situ transmission UV-Vis spectroscopy were performed after film deposition.

[1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017),
[2] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).

CPP 58.5 Wed 17:30 H 0111

Anomalous Roughness Evolution of Organic Mixed Films — ●ALEXANDER HINDERHOFER, JAN HAGENLOCHER, MARTIN OETTEL, and FRANK SCHREIBER — Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

The surface morphology and roughness of thin films and crystals depend on competing mechanisms, which either roughen or smooth the film surface during growth. Important roughening mechanisms, are kinetic roughening based on shot noise and roughening due to mound growth, which is facilitated by reduced interlayer transport, often associated with a step edge. While these issues have been well studied for growth of simple atomic species, comparatively little is known about organic systems. These are expected to exhibit a fundamentally different growth behavior, due to their different interactions (van-der-Waals) and thus different response to strain and due to their internal degrees of freedom.

We use in situ x-ray reflectivity and complementary atomic force microscopy to monitor crystallinity and roughness evolution during growth of organic binary mixtures of several compounds, i.e. pentacene (PEN), perfluoropentacene (PFP), diindenoperylene (DIP) fullerene (C60). A general trend of reduced roughness in the mixed films compared to the pure materials is observed. We will discuss this roughness evolution in relationship to the in-plane crystallinity of the thin films and will show that the growth behavior can be rationalized by a, compared to homoepitaxy, lowered step edge barrier for lower in-plane crystallinity.

CPP 58.6 Wed 17:45 H 0111

Grain boundaries and charge carrier diffusion in large crystal MAPI thin films — ●RICHARD CIESIELSKI¹, FRANK SCHÄFER¹, NICOLAI HARTMANN¹, NADJA GIESBRECHT¹, THOMAS BEIN¹, PABLO DOCAMPO², and ACHIM HARTSCHUH¹ — ¹Department Chemie und Center for Nanoscience (CeNS), LMU München, Deutschland — ²School of Electrical and Electronic Engineering, Newcastle University, United Kingdom

Micro- and nanocrystalline methyl-ammonium lead-iodide (MAPI)-based thin film solar cells today reach power conversion efficiencies

of up to 20%. We investigate the impact of grain boundaries on charge carrier transport in large crystal MAPI thin films using time-resolved photoluminescence (PL) microscopy and numerical model calculations. While long-ranged diffusive charge carrier transport is observed within single crystals, no transport occurs across the grain boundaries. The observed PL transients are found to crucially depend on the microscopic geometry of the crystal and the point of observation. Our experimental results show no quenching or additional loss channels due to grain boundaries for the studied material, which thus do not negatively affect the performance of derived thin film devices.

CPP 58.7 Wed 18:00 H 0111

Nanoporous thin films of organic semiconductors for gas sensing applications — •JEAN-NICOLAS TISSERANT, WOLFGANG KOWALSKY, and ROBERT LOVRINCIC — TU Braunschweig, Institut für Hochfrequenztechnik c/o InnovationLab, Speyerer Str. 4 69115 Heidelberg

Organic semiconducting devices could find applications in high added-

value products such as efficient sensors for the detection of toxic gases.(1) Nanoporous morphologies are particularly interesting in this scope because they offer enhanced interfacial areas compared to the corresponding planar materials. Processes such as the diffusion of an analyte molecule to the active area of a gas sensor (2) may thus be improved proportionally to the amount of interface added. We propose to use nanoporous thin films of semiconductors in an organic field-effect transistor (OFET) for sensing of an endocrine disruptor in air. In the strategy that we follow, organic semiconducting molecules were self-assembled into nanoporous 2D films following a recently developed method.(3,4) These films were biased in an OFET configuration to build an indirect sensor in which the non-covalent interaction between a sensing dielectric and the target molecule modifies the electrical characteristics of the transistor.

References: (1)Zhang, C., Chen, P. & Hu, W. Chem. Soc. Rev. 44, 2087-2107 (2015); (2)Zhang, F., Qu, G., Mohammadi, E., Mei, J. & Diao, Y. Adv. Funct. Mater. 27, 17-20 (2017); (3)Tisserant, J. N. et al. RSC Adv. 6, 23141-23147 (2016); (4)Tisserant, J.-N. et al. ACS Appl. Mater. Interfaces 9, 27166-27172 (2017)