

DS 46: Organic Electronics and Photovoltaics VI (jointly with CPP, HL, O)

Time: Thursday 17:45–19:45

Location: CHE 91

DS 46.1 Thu 17:45 CHE 91

The role of residual additives on the stability of polymer blend materials for organic photovoltaic applications. —

•AURÉLIEN TOURNEBIZE^{1,2}, AGNÈS RIVATON², HEIKO PEISERT¹, and THOMAS CHASSÉ¹ — ¹Institute of Physical and Theoretical Chemistry, Tübingen, Germany — ²Institut de Chimie de Clermont-Ferrand, France

Processing additives for improved the morphology of the bulk heterojunction (BHJ) materials used in organic solar cells (OSCs) is now very popular. Thus, by optimizing the donor and acceptor nano domains, the efficiency of OSCs devices could be significantly increased. [1] The impact of those additives on the performances has been widely explored recently but nothing in terms of stability. And yet, a part of the additives stays trapped in the thin film [2] and could participate in the complex photodegradation of the polymer blend materials.

In the present work, we have investigated the impact of residual additives on the polymer blend photostability. By using essentially spectroscopic technics, we have observed an acceleration of the polymer blend photodegradation in presence of additives. In this context, the use of new additives providing a better morphology and by the way a better stability was also explored.

[1] J.K. Lee, W.L. Ma, C.J. Brabec, J. Yuen, J.S. Moon, J.Y. Kim, K. Lee, G.C. Bazan, and A.J. Heeger JACS. 2008, 130, 3619-3623 [2] L. Ye, Y. Jing, X. Guo, H. Sun, S. Zhang, M. Zhang, L. Huo, and J. Hou J. Phys. Chem. C 2013, 117, 14920-14928

DS 46.2 Thu 18:00 CHE 91

Electronic States and Electrochemical Properties of Polymeric Phthalocyanine Sheets —

•CLEMENS GEIS and DERCK SCHLETTWEIN — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Phthalocyanines are forming organic semiconducting thin films applicable in field-effect transistors, organic solar cells and as heterogeneous chemical catalysts. They consist of a planar organic aromatic ligand around a central metal atom like *Cu*, *Fe* or *Co*. In a chemical vapour deposition reaction (CVD) phthalocyanines with polymerized ligands were synthesized by reactions of bifunctional 1,2,4,5-tetracyanobenzene with thin metal films. By these means a high concentration of the catalytically active metal-sites on the substrate is established, they are electronically coupled and a molecular network is formed by such sheet polymers. Photoelectron spectroscopy was used to characterize the electronic states of the metals and ligands. Metal ions in the complexes as well as neutral metal clusters were detected in the films. Optical transmission spectroscopy was used to discuss the uniformity of the electronic excitation energy and its dependence on preparation conditions. The films were electrochemically reduced and oxidized to further study their accessible electronic states, study consequences for their optical absorbance and to test the polymeric phthalocyanines as electrocatalysts for water oxidation to oxygen and reduction to hydrogen, reactions of highest interest for the chemical storage of electrical energy from fluctuating renewable sources.

DS 46.3 Thu 18:15 CHE 91

Asymmetry of mixing length scales and kinetics of phase-separation in co-evaporated donor-acceptor organic thin film blends —

•RUPAK BANERJEE, CHRISTOPHER LORCH, ALEXANDER GERLACH, JIŘÍ NOVÁK, CHRISTIAN FRANK, JOHANNES DIETERLE, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Small molecular organic semiconductors have found widespread usage in organic photovoltaics (OPV) due to their attractive optical, structural and electronic properties [1]. One of the many ways to tune the efficiency of an OPV is by mixing donor (D) and acceptor (A) materials [1] since the efficiency depends on the interplay of the diffusion lengths of the excitons generated by the absorption of light and the structural length scales of the D:A mixture. Controlling the structural length scales in D:A mixtures is thus of paramount importance [2]. We discuss *in situ* and real-time x-ray scattering studies on the structure of mixed D:A films as a function of mixing ratio which reveal the kinetics and thickness dependence of phase separation and in particular the asymmetry between top and bottom interfaces [3]. We further discuss the influence of interrupted growth on the phase-separation kinetics of

such systems.

[1] W. Brütting and C. Adachi, Physics of Organic Semiconductors, Wiley-VCH, Weinheim (2012).

[2] A. Opitz *et al.*, IEEE J. Sel. Top. Quant. **16**, 1707 (2010).

[3] R. Banerjee, J. Novák, C. Frank, C. Lorch, A. Hinderhofer, A. Gerlach, and F. Schreiber, Phys. Rev. Lett. **110**, 185506 (2013).

DS 46.4 Thu 18:30 CHE 91

UPS studies on different air-stable molecular n-dopants —

•MARTIN SCHWARZE¹, MAX L. TIETZE¹, PAUL PAHNER¹, BEN NAAB², ZHENAN BAO², BJÖRN LÜSSEN¹, DANIEL KASEMANN¹, and KARL LEO¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — ²Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States

Understanding the working mechanism of electrical doping in organic semiconductors is essential for the optimization of organic semiconductor devices. A defined doping level allows for the control of the Fermi level position and the conductivity of transport layers. In comparison to molecular p-doping of organic semiconductors, n-doping has the additional problem of air instability. To successfully transfer an electron to the lowest unoccupied molecular orbital (LUMO) of the matrix material, dopants exhibiting shallow highest molecular orbitals (HOMO) are necessary, rendering them prone to reactions with e.g. oxygen. In this study, three different types of n-dopants are compared, an air stable cationic DMBI and DMBI dimer with the air sensitive W2(hpp)4. Doping efficiency, Fermi-level shift, air stability, and conductivity at different doping concentrations are investigated by ultraviolet photoelectron spectroscopy (UPS) and electrical measurements.

DS 46.5 Thu 18:45 CHE 91

Fracture and corrosion protection for thin-film encapsulation

- **Fine-tuning the electrical calcium corrosion test for water vapor permeation measurements** — •FREDERIK NEHM, HANNES KLUMBIES, LARS MÜLLER-MESKAMP, and KARL LEO — Institut für Angewandte Photophysik, TU Dresden, Dresden, Deutschland

In recent years, the demand for ultra-high moisture barriers has strongly increased due to the ongoing development of organic electronics. Thus, the ability to measure water vapor transmission rates (WVTRs) below $10^{-5} \frac{g(H_2O)}{m^2d}$ - less than a monolayer in 10 days - is crucial for barrier development. The electrical calcium corrosion test - monitoring the decreasing conductivity of a thin calcium film turning into calcium hydroxide - is a sensitive, cost-efficient method to measure such low WVTRs. However, poor design can cause a high background rate or test breakdown. We show that calcium corrosion causes barrier breaking by both expansion and hydrogen emission. As a countermeasure, we introduce organic (C₆₀) buffer layers for decoupling on both sides of the calcium film. Further investigations show elevated calcium corrosion at the calcium-electrode-interface which can be prevented by a proper choice of the electrode material. Finally, the massive corrosion of barrier thin films is shown to be prevented by glueing a polymer foil onto the barrier under testing. With these precautions, we show atomic layer deposited alumina barriers measured in thin film encapsulation structure close to an actual device architecture. At 30°C, 90% rh, WVTRs of below $5 \cdot 10^{-5} \frac{g(H_2O)}{m^2d}$ were obtained.

DS 46.6 Thu 19:00 CHE 91

Commensurability as the determining factor for molecular tilt and multilayer growth: In-situ and real-time growth study of the nanographene HBC on SiO₂ and HOPG —

•PAUL BEYER¹, TOBIAS BREUER², SALIOU NDIAYE², ANTON ZYKOV¹, ANDREAS VIERTTEL¹, MANUEL GENSLE¹, JÜRGEN P. RABE¹, STEFAN HECHT¹, GREGOR WITTE², and STEFAN KOWARIK¹ — ¹HU Berlin, 12489 Berlin — ²Philipps-Universität Marburg, 35032 Marburg

We investigate the influence of symmetries and the substrate-molecule commensurability on the structure and growth kinetics of the nanographene hexa-*peri*-hexabenzocoronene (HBC). We study organic molecular beam deposited ultrathin HBC films on SiO₂, pristine and sputtered HOPG because of the similar surface energies, singling out the influence of the lattice-matching between HBC and graphite. Using real-time and *in situ* x-ray growth oscillations we find the first ad-layer to grow lying down on both substrates. On pristine HOPG we find a superstructure of hexagonally arranged, recumbent molecules

in a new polymorph using GIXD, XRR and NEXAFS. The loss of commensurability in the sputtered HOPG leads to mainly upright molecules. Equally, we find a transition to upright molecules on amorphous SiO₂ surfaces. On SiO₂ micro-crystallites in the bulk structure that completely cover the substrate are found, while the strong ordering on HOPG leads to island growth of the new polymorph as observed by AFM. Our results demonstrate that the (lack of) symmetry- and lattice-matching critically determines the molecular orientation and occurrence of surface induced polymorphs.

DS 46.7 Thu 19:15 CHE 91

Spray coating process for highly conductive silver nanowire networks as transparent top electrode for small molecule organic photovoltaics — •FRANZ SELZER¹, NELLI WEISS², DAVID KNEPPE¹, LUDWIG BORMANN¹, CHRISTOPH SACHSE¹, NIKOLAI GAPONIK², LARS MÜLLER-MESKAMP¹, ALEXANDER EYCHMÜLLER², and KARL LEO¹ — ¹IAPP, TU Dresden — ²Phy. Chem., TU Dresden

Organic photovoltaics are a promising technology for fabrication in high throughput R2R-coating machines. Therefore, flexible and highly conducting transparent electrodes on temperature sensible polymer films are required. Percolative networks made of silver nanowires (AgNWs) are a flexible alternative, showing an opto-electrical performance comparable to ITO. Usually, they are deposited from solution, followed by post-annealing (200°C). The solvents involved in the deposition limit the versatility of this type of electrode and do not allow the direct deposition as top contact onto evaporated small molecule de-

vices. Here, we present a novel spray-coated AgNW mesh, showing excellent opto-electrical performance although processed below 80°C. We investigate different types of wire functionalization and the consequences on typical network parameters of AgNWs. By comparing all investigated materials for different parameters like varying concentration and by scanning electron microscopy, the basics of the sheet resistance reduction mechanism are extracted and AgNW electrodes (<50Ohm/sq@>80%) are processed at 30°C. Finally, the successful implementation as transparent top electrode for high-performance organic p-i-n type solar cells is demonstrated.

DS 46.8 Thu 19:30 CHE 91

Tuning the energy levels of carbon nanotubes by functionalization — •GERHARD LACKNER¹, WEI XIA², VLADIMIR SHVARTSMAN¹, MARTIN MUHLER², and DORU C. LUPASCU¹ — ¹Institute for Materials Science, University of Duisburg-Essen, 45141 Essen, Germany — ²Laboratory of Industrial Chemistry, Ruhr-University Bochum, 44801 Bochum, Germany

Carbon nanotubes (CNT) are a promising material for electrical applications due to their extraordinary properties. Nevertheless, a defined tuning of the energy levels of this material has not been reported so far. We show a possible route to set the energy levels of CNT by functionalization. The energy levels before and after the functionalization are analysed by Kelvin Probe measurements. Additionally, the functionalized and non-functionalized CNT are applied in organic solar cells and a comparative study about the solar cell performances is given.