O 32: [DS] Organic electronics and photovoltaics: simulations and optics II (jointly with CPP, HL, O)

Time: Tuesday 11:30–13:00 Location: H 2032

O 32.1 Tue 11:30 H 2032

Fast, stable and high-brightness light-emitting electrochemical cells — •Sebastian B. Meier^{1,2}, Daniel Tordera³, Henk J. Bolink³, Wiebke Sarfert², and Albrecht Winnacker¹ — ¹University of Erlangen-Nuremberg, Department of Materials Science, Chair VI: Materials for Electronics and Energy Technology, Erlangen, Germany — ²Siemens AG, Corporate Technology, GTF Organic Electronics, Erlangen, Germany — ³Instituto de Ciencia Molecular, Universitat de València, Paterna, Spain

Light-emitting electrochemical cells (LECs) are among one of the simplest class of light-emitting devices based on organic semiconducting materials. In its most facile form they just comprise a single solutionprocessed layer of an ionic transition metal complex (iTMC) sandwiched between two air-stable electrodes, which supports all the three events of charge injection, charge transport and radiative recombination. The ordinary architecture and the possibility to use stable electrode materials is a direct consequence of the ionic nature of the active layer enabling efficient charge injection with concomitant in-situ electrochemical doping resulting in the formation of a light-emitting p-i-n junction. There has been a longstanding issue in iTMC device operation between fast response and high stability when standard constant DC voltage is used, which is due to the dynamic nature of the junction. We will show how to stabilize the dynamic junction to achieve long-living (> 1000 h) high-brightness (> 1200 cd/m²) iridium(III) iTMC-based LECs possessing simultaneous fast turn-on times (< 20s) at considerable light intensity ($> 200 \text{ cd/m}^2$).

O 32.2 Tue 11:45 H 2032

Charge Carrier Storage on Emitter Molecules in Organic Light-Emitting Diodes — ◆CAROLINE WEICHSEL¹, SEBASTIAN REINEKE¹,², BJÖRN LÜSSEM¹, and KARL LEO¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, D-01069 Dresden, Germany — ²Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

In this contribution, we study trapping of charge carriers in phosphorescent organic light-emitting diodes (OLED) using the red emitter iridium(III)bis(2-methyldibenzo[f,h]quinoxaline) (acetylacetonate) [Ir(MDQ)2(acac)] by transient electroluminescence. We observe a transient overshoot exceeding regular light emission after voltage turnoff, which can be explained by delayed charge carrier recombination of charges stored in the emission layer. We study this mechanism by variation of the off-voltage and by adding thin quenching layers, which allow to determine the position of the emission zone during regular light emission and after voltage turn-off. Additionally, we show that the signal intensity is linearly proportional to the doping concentration. Investigations on the applied current and the pulse length show a saturation of the overshoot intensity, which we ascribe to the limited ability of emitter molecules to store electrons. We propose that this storage process negatively affects the external quantum efficiency of the OLED. We assume that the effect can also take place in other OLED structures and suggest that the methods presented here can help identifying charge carrier storage on emitter molecules.

O 32.3 Tue 12:00 H 2032

Surface Modification Effect on Optical Anisotropy and Molecular Orientation of CuPc Thin Films — •L. Ding, M. Friedrich, O. Gordan, and D. R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Copper phthalocyanine (CuPc), as an organic semiconductor, attracts much attention currently due to its potential application in organic electronic and photovoltaic devices. Molecular orientation plays a significant role to improve the device performance. In situ spectroscopic ellipsometry (SE) and reflection anisotropy spectroscopy (RAS) are employed simultaneously to investigate the out-of-plane and in-plane anisotropy as well as molecular orientation of CuPc thin films, respectively.

Chemically prepared octade cyltrichlorosilane (OTS) monolayer with upright standing molecules shows a significant influence on the out-of-plane anisotropy with an average out-of-plane tilt angle of 69.3° +/- 4.1° but little impact on the in-plane anisotropy. Nearly flat lying CuPc molecules are observed on thermally evaporated Perylene-3,4,9,10-tetracarboxylic-3,4,9,10-dianhydride (PTCDA) layers thicker than 3.4 nm, giving an average tilt angle of 19.7° +/- 8.0° due to the flat lying PTCDA molecules on Si. Meanwhile, the in-plane anisotropy of CuPc is much lower than that without PTCDA. The influence of the PTCDA layer thickness on molecular orientation can be explained by the island growth mode of PTCDA.

O 32.4 Tue 12:15 H 2032

Stability of perfluroro-pentacene thin films on coinage metals — \bullet Christian Schmidt¹, Tobias Breuer¹, Stefan Wippermann², Wolf Gero Schmidt², and Gregor Witte¹ — 1 Molekulare Festkörperphysik, Philipps-Universität Marburg, Germany — 2 Theoretische Physik, Universität Paderborn, Germany

The development of organic electronics greatly benefits from the systematic improvement of molecular properties by chemical functionalization. One example constitutes pentacene that can be prevented from oxidization by perfluorination. Topical investigations of the interface properties of perfluoropentacene (PFP) are frequently conducted only from an electronic point of view, measuring either macroscopic device properties or valence band spectra. In these studies possible chemical interactions have not been addressed since PFP is especially designed to be more stable than PEN. It was therefore unexpected that PFP monolayers on Cu(111) undergo degradation upon heating and that decomposition also occurs on Ag(111). This means that PFP is less stable than PEN, which desorbs intact from Ag(111). This behaviour is especially remarkable when considering that PFP is farther above metal surfaces than PEN. This unclear situation is very problematic, as the PFP-metal interface itself serves as a model system for electronic effects and is of vital interest in this field. Therefore, we systematically studied the thermal behaviour of PFP on the coinage metals by means of temperature NEXAFS and XPS. In order to understand underlying mechanisms we accompany our experimental data with density functional theory (DFT) calculations including chemical reactions.

O 32.5 Tue 12:30 H 2032

Two dimensional band structure mapping of organic single crystals using the new generation electron energy analyzer ARTOF — •A. Vollmer¹, R. Ovsyannikov¹, M. Gorgot¹, S. Krause¹, M. Oehzelt¹, N. Martensson², S. Svensson², P. Karlsson³, M. Lundquist³, J. Pflaum⁴, T. Schmeiler⁴, and N. Koch¹,⁵ — ¹Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — ²Uppsala University, Uppsala, Sweden — ³VG Scienta, Uppsala, Sweden — ⁴Universität Würzburg, Würzburg, Germany — ⁵Humboldt-Universität zu Berlin, Berlin, Germany

We report on a novel type of photoemission instrument, the Angle Resolved Time Of Flight analyzer (ARTOF 10k)electron energy analyser. The instrument facilitates the simultaneous recording of kinetic energy and angular pattern of photoelectrons in a cone of up to 30° opening angle with very high energy resolution (100 μ eV). Its transmission (250 times higher than in hemispherical analysers) allows for very mild conditions during the experiment turning the ARTOF into the predestined instrument to investigate sensitive specimens such as organic single crystals, as extremely low photon fluxes can be used. Even though organic single crystals are of increasing fundamental and applied scientific interest, knowledge of their electronic properties is still mainly based on theoretical calculations due to major experimental challenges in measuring photoemission. Here we present the band structures of rubrene and tetracene single crystals obtained with unprecedented quality using the ARTOF instrument within only a few hours of measurement time.

O 32.6 Tue 12:45 H 2032

Electronic structure of prototypical organic-organic heterojunctions for photovoltaic applications — \bullet Andreas Wilke¹, Raphael Schlesinger¹, Ullrich Hörmann², Jens Niederhausen¹, Johannes Frisch¹, Antje Vollmer³, Julia Wagner², Mark Gruber², Andreas Opitz¹, Wolfgang Brütting², and Norbert Koch^{1,3} — ¹Humboldt-Universität zu Berlin — ²Universität Augsburg — ³Helmholtz-Zentrum Berlin für

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In organic photovoltaic cells (OPVCs) typically two organic materials with electron acceptor and donor character are sandwiched between anode and cathode, forming either layered planar (PHJ) or bulk heterojunctions, where charge separation occurs. We report ultraviolet photoelectron spectroscopy (UPS) measurements done for three different organic-organic PHJs, comprising the donors sexithiophene (6T) and poly(3-hexylthiophene) (P3HT), and the acceptors diindenoperylene (DIP) and C60. The respective heterojunctions were formed on

poly(ethylenedioxythiophene): poly(styrenessulfonate) (PEDT:PSS) electrodes. The energy level alignment found experimentally for these heterojunctions are discussed in relationship to the open circuit voltages achieved in corresponding PHJ OPVCs. The offset between the highest occupied molecular orbital of the donor and the lowest unoccupied molecular orbital of the acceptor, an estimate for the maximum achievable open circuit voltage, peaked at 1.75 eV for the 6T/DIP PHJ. In actual OPVCs based on 6T/DIP, an open circuit voltage of up to 1.38 V was observed.