

## CPP 13: Organic Electronics and Photovoltaics - Hybrid and Organic Layer Systems

Time: Monday 15:00–16:30

Location: C 243

CPP 13.1 Mon 15:00 C 243

**Electrical characterization of hybrid n-GaN/p-PEDOT structures for optoelectronic applications** — •LINUS KRIEG<sup>1</sup>, DANIEL SPLITH<sup>2</sup>, ZHIPENG ZHANG<sup>2</sup>, HOLGER VON WENCKSTERN<sup>2</sup>, MARIUS GRUNDMANN<sup>2</sup>, FLORIAN MEIERHOFER<sup>1</sup>, XIAOXUE WANG<sup>3</sup>, KAREN GLEASON<sup>3</sup>, and TOBIAS VOSS<sup>1</sup> — <sup>1</sup>Institute of Semiconductor Technology and Laboratory for Emerging Nanometrology, Braunschweig University of Technology, 38092 Braunschweig — <sup>2</sup>Felix-Bloch-Institut für Festkörperphysik, Halbleiterphysik, Linnéstr. 5, 04103 Leipzig — <sup>3</sup>Department of Chemical Engineering, Massachusetts Institute of Technology, 02139 Cambridge

Hybrid structures consisting of both inorganic and organic conductive layers are promising for the development of inexpensive, versatile and tailored electronic and optoelectronic devices such as sensors or light emitting diodes (LEDs). We study the fabrication of planar n-GaN/p-PEDOT heterostructures. The p-polymer is grown via oxidative chemical vapor deposition (oCVD), a dry deposition approach that allows for controllable polymer deposition out of the gas phase while achieving conformal coverage of the substrate with a thickness control of the deposited polymer layer in the nanometer range. We analyze the temperature-dependent current-voltage characteristics of the hybrid GaN/PEDOT-structures to study the electronic properties of the hybrid interface. The results show a pronounced diode characteristic of the hybrid device and allow us to deduce the relevant conduction mechanisms. We deduce the saturation current of the device and develop a model of the band lineup hybrid n-inorganic/p-organic interface.

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**Bias dependency of hybrid charge transfer emission at planar ZnO/small molecule interfaces** — •STEFAN ZEISKE<sup>1</sup>, ULRICH HÖRMANN<sup>1</sup>, FORTUNATO PIERSIMONI<sup>1</sup>, LUKAS HOFFMANN<sup>2</sup>, THOMAS RIEDL<sup>2</sup>, DENIS ANDRIENKO<sup>3</sup>, and DIETER NEHER<sup>1</sup> — <sup>1</sup>Universität Potsdam, Germany — <sup>2</sup>Bergische Universität Wuppertal, Germany — <sup>3</sup>MPI Mainz, Germany

Recent studies propose that the electroluminescence from hybrid charge transfer excitons (HCTX) depends not only on the interfacial energy gap but also on the applied bias. The models to explain these observation base either on filling of trap states, or on the assumption of delocalized HCT state confined in a triangular quantum well created by the electric field. Here, we investigate the origin of the bias dependent HCTX emission at planar interfaces between the ZnO and different small molecules. We find a nearly linear dependency of the EL peak position on the applied electric field. The independency of the slope on the organic layer thickness confirms that the shift is caused by a field and reminds of the linear Stark effect. Simple 1D quantum mechanical models confirm this interpretation and predict a moderate hole delocalization in the organic of the order of the typical size of a small molecule. Electrostatic treatment of the interaction of the charged molecule with its image potential, however, reveals that the observed field dependence is considerably influenced by the polarizability of the organic cation. As a direct consequence the field-induced shift of the EL peak is expected to be strongly dependent on the molecular orientation at the hybrid interface.

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**Energetics of polar organic metal-insulator-semiconductor diodes probed by different techniques** — •ALEXANDER HOFMANN<sup>1</sup>, SIMON ZÜFLE<sup>2</sup>, STÉPHANE ALTAZIN<sup>2</sup>, KOHEI SHIMIZU<sup>3</sup>, BEAT RUHSTALLER<sup>2</sup>, HISAO ISHII<sup>3</sup>, and WOLFGANG BRÜTTING<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — <sup>2</sup>Institute of Computational Physics, ZHAW, 8401 Winterthur, Switzerland — <sup>3</sup>Center for Frontier Science, Chiba University, Chiba, 263-8522 Japan

The strong dipole moment of polar organic materials like tris-(8-hydroxyquinolate) aluminum (Alq<sub>3</sub>), if not oriented perfectly anisotropic, will lead to the buildup of a giant surface potential (GSP) of the organic film. As we have shown previously [1], it is possible to apply the CELIV (Charge Extraction by Linearly Increasing Voltage) method on polar diodes to determine the charge transport activation energy. Combined with impedance spectroscopy, this technique can be used to measure the injection barrier of the underlying metal-

semiconductor interface [2]. In this contribution, we show the practical performance of this method compared to ultra violet photoelectron spectroscopy as an established method of determining injection barriers. We have applied the technique to the prototypical polar organic system *N,N'*-Di(1-naphthyl)-*N,N'*-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) and Alq<sub>3</sub> in different dilutions and show the dependence of the determined barrier on the dilution ratio.

[1] Journal of Applied Physics **121**, 175501 (2017) [2] Journal of Applied Physics **122**, 115502 (2017)

CPP 13.4 Mon 15:45 C 243

**Theoretical determination of the ionization potential and the electron affinity of organic semiconductors** — •SUSUMU YANAGISAWA — University of the Ryukyus

Ionization potential (IP) and electron affinity (EA) of organic semiconductors are important quantities, which are relevant to barriers for injection of charge (hole or electron). The electrostatic and electronic polarization contributions to the polarization energies for the injected charges in pentacene polymorphs were investigated with first-principles calculations. The former contribution was estimated by employing periodic slabs of the surfaces at the semi-local density functional level of theory. On the other hand, the latter was treated for the bulk systems at the many-body perturbation theory within the GW approximation. It was found that while the electronic polarization induced narrowing of the energy gap in the single crystal and the thin film phases, the electrostatic effect shifted up or down the frontier energy levels such as the highest-occupied molecular orbital- (HOMO) and the lowest-unoccupied molecular orbital-derived (LUMO) levels relative to the vacuum level, sensitively to the molecular orientation at the surface. The role of the electrostatic interaction such as the charge-permanent quadrupole interaction dominating IP and EA of the materials is discussed.

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**Hot electrons and hot spins at metal-organic interfaces** — •THORSTEN ARNOLD<sup>1</sup>, AINHOA ATXABAL<sup>2</sup>, SUBIR PARUI<sup>2</sup>, LUIS E. HUESO<sup>2</sup>, and FRANK ORTMANN<sup>1</sup> — <sup>1</sup>Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany — <sup>2</sup>CIC nanoGUNE, 20018 Donostia-San Sebastian, Basque Country, Spain

Metal-organic barriers between the metal Fermi energy and the molecular levels of the organic semiconductor play a fundamental role in the performance of organic electronic devices. In order to measure these barriers, recently, a hot-electron transistor device has been developed [1]. We propose a theoretical model [2], which describes all the transport effects of the hot electrons for the first time. The model is able to reproduce the experimental results with excellent accuracy.

The model is extended to predict the transport characteristics of spin-polarized hot electrons in these devices. We find a spatial variation of the spin diffusion length, which scales inversely proportional to the variation of the electron density. The spin current can be increased by increasing the hot electron energy and by decreasing the image charge barrier without changing the spin diffusion length. We also provide unprecedented insight into the effects of disorder at the metal-organic interface. Finally, we establish conditions when pure spin currents appear, where majority and minority spin carriers propagate in opposite directions.

[1] A. Atxabal et al., Adv. Mater. **29**, 1606901 (2017).

[2] T. Arnold et al., Adv. Funct. Mater. (to be published).

CPP 13.6 Mon 16:15 C 243

**Exciting Strong Fano Resonances by Stacking Plasmonic Nanostructures** — •YE YU<sup>1</sup>, ZIWEI ZHOU<sup>2</sup>, TOBIAS A. F. KÖNIG<sup>1,3</sup>, and ANDREAS FERY<sup>1,3,4</sup> — <sup>1</sup>Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Straße 6, 01069, Dresden, Germany — <sup>2</sup>State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun, China — <sup>3</sup>Cluster of Excellence Centre for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany — <sup>4</sup>Department of Physical Chemistry of Polymeric Materials, Technische Universität Dresden, Hohe Str. 6, 01069 Dresden, Germany

Small gaps at nanometer-scale enabled noble metals to be perfect re-

search of interest in the field of plasmonic sensing devices, optical antennas, and nanolasing systems. Due to the ultra-small gap formed in between two metallic components, the coupling effect is usually enormous and hence extreme nanoscale confinement and enhancement of the near electric field intensity. Despite the huge potential in these nanogap devices, challenges still remain in manufacturing the advanced devices with high throughput and reproducibility. Here we propose to

fabricate nanogap structures with a combination of bottom-up assembly and top-down patterning strategy in the mean of lower cost and higher throughput. We were able to fabricate nanogap structures of high quality and also over large area. The optical properties proven to be of high electric field enhancement with the possibility of exciting Fano resonances due to the plasmonic hybridization between two metallic parts forming the nanogaps.