

## CPP 36: Focus: Exploitation of Anisotropy in Organic Semiconductors I (joint session CPP/HL)

Molecular glasses and semi-crystalline thin films play a key role in organic semiconductor devices, particularly organic light-emitting diodes and solar cells. Surprisingly, some of these materials exhibit considerable anisotropies regarding their molecular orientation which leads to non-isotropic electronic properties. In spite of the importance for optoelectronic devices, however, this phenomenon is not fully understood yet. This focus session will bring together concepts from the physics of glasses, structure formation in soft matter as well as applications of such anisotropic molecular solids in organic electronics. Organized by: Wolfgang Brütting (University Augsburg), Sebastian Reineke (TU Dresden); Wolfgang Wenzel (Karlsruher Institut für Technologie).

Time: Tuesday 10:00–12:30

Location: ZEU 222

### Invited Talk CPP 36.1 Tue 10:00 ZEU 222

**Anisotropic packing in vapor-deposited glasses** — ●MARK EDIGER — University of Wisconsin-Madison, USA

Glasses are generally regarded as highly disordered and the idea of controlling molecular packing in glasses is reasonably met with skepticism. However, as glasses are non-equilibrium materials, a vast array of amorphous structures are possible in principle, even for a single component system. Physical vapor deposition (PVD) allows a surprising amount of control over anisotropic molecular packing in glasses. For organic semiconductors, glasses can be prepared in which the molecules have a substantial tendency to stand-up or lie-down relative to the substrate, and molecular layering can also be achieved. The high density and anisotropic packing of PVD glasses can be explained by a mechanism that is "anti-epitaxial" as structure is templated by the top surface rather than by the underlying substrate. This mechanism implies that similar structures can be prepared by increasing substrate temperature and by decreasing deposition rate, and this has recently been experimentally verified.

### CPP 36.2 Tue 10:30 ZEU 222

**Clarifying the orientation mechanism of homoleptic Iridium-carbene complexes** — ●MARKUS SCHMID<sup>1</sup>, KRISTOFFER HARMS<sup>2</sup>, THOMAS MORGENSTERN<sup>1</sup>, ALEXANDER HOFMANN<sup>1</sup>, HANS-HERMANN JOHANNES<sup>2</sup>, WOLFGANG KOWALSKY<sup>2</sup>, and WOLFGANG BRÜTTING<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — <sup>2</sup>Institute for high frequency technology, TU Braunschweig, 38106 Braunschweig, Germany

Horizontal orientation of the emitting species is one of the most promising techniques to increase the efficiency of state of the art organic light emitting diodes. Especially metal-organic compounds have attracted great attention. While the alignment has been observed and explained for many heteroleptic Iridium complexes, there has been less progress for their homoleptic counterparts. Only few homoleptic compounds have been reported to show a beneficial morphology in guest-host systems. In this study, we investigated multiple derivatives and isomers of the sky-blue dye tris(*N*-dibenzofuran-*N'*-methylimidazole)iridium(III) (Ir(dbfmi)<sub>3</sub>) doped in the hosts Bis[2-(diphenylphosphino)phenyl]ether oxide (DPEPO) and 3,6-bis(diphenylphosphoryl)-9-phenylcarbazole (PO9). By a combination of optical techniques to probe the transition dipole orientation and electrical measurements to access the permanent dipole moment, we revealed that this homoleptic complex is significantly aligned in both matrices. From our insights into the film morphology we postulate that an anisotropic interaction is responsible for the orientation and even identified the region of the molecule that causes this behavior.

### CPP 36.3 Tue 10:45 ZEU 222

**Application of polar molecules to electret for vibrational energy generator: Improvement of device productivity and output power by utilizing spontaneous orientation polarization** — ●YUYA TANAKA<sup>1,2</sup>, NORITAKA MATSUURA<sup>1</sup>, and HISAO ISHII<sup>1</sup> — <sup>1</sup>Chiba University, Chiba, Japan — <sup>2</sup>Japan Science and Technology Agency, PRESTO, Saitama, Japan

Electret-based vibrational energy generator (E-VEGs) have attracted much attention because they can generate electrical power from ambient vibrations. The challenges for E-VEGs are to: (i) simplify charging process for making electret and (ii) enhance output power (P) of the device. Recently, we developed polar molecules (PM), such as Alq3 and TPBi, based VEGs that do not require any charging process by utilizing spontaneous orientation of the molecules. To increase P of

the device, enhancement of surface potential (SP), namely, order parameter of the molecule, is required. In this study, we prepared PM films with various deposition rate (r). We found that the SP becomes larger in the case of high r, suggesting that molecular orientation can be controlled by r. Further, the estimated surface charge density was comparable to conventional polymer-based electret after charging (typically, 2 mC/m<sup>2</sup>). We believe that the realization of PM-VEGs will open up the novel ways for supplying electrical energy to the various devices.

### CPP 36.4 Tue 11:00 ZEU 222

**Post processing temperature dependence of the emitter molecule orientation in organic thin films** — ●CHRISTIAN HÄNISCH, SIMONE LENK, and SEBASTIAN REINEKE — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Germany

One of the main loss channels reducing the efficiency of organic light-emitting diodes is optical trapping of already generated photons due to total internal reflection and coupling to plasmonic modes. Aligning the transition dipole moment of the emitter molecules parallel to the interface planes of the stratified device structure can drastically decrease the unusable power fraction.

In this work, the long term, post processing stability of the molecular orientation of two well-known phosphorescent emitters is investigated for different storage temperatures up to 95% of the glass transition temperature (T<sub>g</sub>) of the host material. Both, photoluminescent samples and electroluminescent devices are analyzed. In the first case, the emission layers are embedded between two layers of higher T<sub>g</sub> in order to avoid crystallization of bare emission layers.

It is shown that the orientation keeps unchanged for several months as long as T<sub>g</sub> is not exceeded but changes immediately as soon as the samples are exposed to temperatures above T<sub>g</sub> for only a few minutes. The latter is demonstrated exemplarily for selected samples after the long term storage period.

### 15 min. break

### Invited Talk CPP 36.5 Tue 11:30 ZEU 222

**Influence of stability and molecular orientation on the properties of stable glasses** — ●JAVIER RODRÍGUEZ-VIEJO — Physics department, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

Stable glasses have attracted great interest since their discovery in 2007. Their superior behavior, compared to liquid-cooled glasses, includes higher kinetic and thermodynamic stability, higher density, sound velocity and elastic moduli or the modification of the low-temperature properties. The origin of the high thermodynamic and kinetic stability of these vapor-deposited glasses is related to the high mobility of surface molecules that enables them to settle into energetic favorable positions during the deposition process. Besides, depending on the molecular shape PVD glasses exhibit packing anisotropies that depend on the deposition temperature. Although molecular orientation does not seem to play a substantial role in the observed stability enhancement, it can have a significant impact in many properties of vapor-deposited glasses. For instance, we have previously shown that molecular orientation may induce variations of the growth front velocity during the heterogeneous transformation of a glass into the supercooled liquid state. In addition, molecular anisotropy plays a key role in charge and thermal transport. We will describe the impact of

the deposition process and the molecular orientation on the thermal properties and on electronic and heat propagation. We also explore the benefits of using stable glasses grown at temperatures around 85%  $T_g$  to increase device efficiency and operational stability of OLEDs.

CPP 36.6 Tue 12:00 ZEU 222

**Infrared organic light-emitting diodes with horizontally oriented carbon nanotube emitters** — ●CAROLINE MURAWSKI<sup>1,3</sup>, ARKO GRAF<sup>2,3</sup>, JANA ZAUMSEIL<sup>2</sup>, and MALTE C. GATHER<sup>3</sup> — <sup>1</sup>Kurt-Schwabe-Institut Meinsberg — <sup>2</sup>Universität Heidelberg — <sup>3</sup>University of St Andrews, UK

Semiconducting single-walled carbon nanotubes (SWCNT) have shown great potential as electrodes and transport layers in organic light-emitting diodes (OLEDs) and field-effect transistors. Here, we incorporate polymer-wrapped SWCNTs as emitter into OLEDs and achieve narrowband pure infrared emission between 1000 and 1200 nm. Due to the 1D nature of CNTs, the transition dipoles exhibit strong horizontal orientation, which results in an exceptionally high outcoupling efficiency of 49%.

CPP 36.7 Tue 12:15 ZEU 222

**Polarized blue photoluminescence of mesoscopically ordered electrospun non-conjugated polyacrylonitrile nanofibers** —

XIAOJIAN LIAO<sup>1</sup>, ●FRANK-JULIAN KAHLE<sup>2</sup>, BIN LIU<sup>3,4</sup>, HEINZ BÄSSLER<sup>2</sup>, XINGHONG ZHANG<sup>3</sup>, SEEMA AGARWAL<sup>1</sup>, ANNA KÖHLER<sup>2</sup>, and ANDREAS GREINER<sup>1</sup> — <sup>1</sup>Macromolecular Chemistry II, U Bayreuth, Germany — <sup>2</sup>Softmatter Optoelectronics, U Bayreuth, Germany — <sup>3</sup>MOE Key Laboratory of Macromolecular Synthesis and Functionalization, Zhejiang University, P. R. China — <sup>4</sup>School of Energy and Power Engineering, North University of China, China

We demonstrate the fabrication of electrospun fibers from the non-conjugated polymer polyacrylonitrile (PAN) that can be aligned by a simple heat-stretching process. Upon excitation at 340 nm ribbons made from the nanofibres show polarized deep blue luminescence with an anisotropy of 0.37 and a quantum yield of about 0.31. Furthermore, they exhibit room temperature green phosphorescences with a lifetime of about 200 ms as well as a delayed deep blue fluorescence resulting from triplet-triplet annihilation (non-coherent photon upconversion). Wide and small angle X-ray scattering experiments show that the stretched electrospun nanofibers are highly aligned with nearly perfect uniaxial orientation within the fabricated ribbons. This results in mechanical robustness and flexibility, with a high specific tensile strength ( $534 \pm 28$ )  $MPa \cdot cm^3/g$  and toughness ( $79 \pm 7$ )  $J/g$ . The combination of efficient polarized deep blue luminescence, room temperature phosphorescence, TTA, mechanical robustness and flexibility of these fibers opens up new avenues for applications.