

## CPP 27: Composites and Functional Polymer Hybrids

Time: Wednesday 11:30–13:00

Location: H39

CPP 27.1 Wed 11:30 H39

**Polymer - Organic Metal Composites for Waste Heat Recovery** — ●MARIE SIEGERT<sup>1</sup> and JENS PFLAUM<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, University of Würzburg, 97074 Würzburg — <sup>2</sup>ZAE Bayern, 97074 Würzburg

The interest in organic thermoelectrics has greatly gained traction over the last decade due to its great potential in waste heat recovery based on sustainable, low-cost materials. For instance, polymers can be solution processed on industrial scale and display aptly low thermal conductivity, but lack high electrical conductivity due to their inherent disorder. Organic molecular metals, on the other hand, exhibit superior electrical conductivity over a wide temperature range, but the complexity of preparation currently limits scalable applications [1]. Here, we report on an approach utilizing suitable polymers in combination with the p-type organic metal TTT<sub>2</sub>I<sub>3</sub> and the n-type Cu(DCNQI)<sub>2</sub>, thus exploiting the benefits of both material classes. As demonstrated by our preliminary experimental data, these composite materials do not only allow for a controlled variation of the thermoelectric properties via the respective amount of organic metal additive but also show significant improvements with respect to their mechanical integrity upon thermal treatment. The related thermoelectric properties of the composites will be evaluated with regard to their application in thin film based organic thermoelectric generators for waste heat recovery. The Deutsche Bundesstiftung Umwelt (DBU) is acknowledged for financial support.

[1] F. Huewe, A. Steeger, et al. Adv. Mat. 29 (2017) 1605682

CPP 27.2 Wed 11:45 H39

**From spinning to spraying functional materials: structural and thermoelectric properties of gold doped spin-casted and spray-deposited P3HT-based thin films** — ●BENEDIKT SOCHOR<sup>1</sup>, ANNA-LENA OECHSLE<sup>2</sup>, CONSTANTIN HARDER<sup>1,2</sup>, ALEXEI VOROBIEV<sup>3,4</sup>, PETER MÜLLER-BUSCHBAUM<sup>2,5</sup>, and STEPHAN V. ROTH<sup>1,6</sup> — <sup>1</sup>Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — <sup>2</sup>Technical University Munich, Physics Department, James-Franck-Str. 1, 85748 Garching, Germany — <sup>3</sup>Institut Laue-Langevin, 71 Avenue des Martyrs, 38042 Grenoble Cedex 9, France — <sup>4</sup>Uppsala University, Department of Physics and Astronomy, Lägerhyddsvägen 1, 752 37 Uppsala, Sweden — <sup>5</sup>Research Neutron Source Heinz Maier-Leibnitz, FRM II, Lichtenbergstr. 1, 85748 Garching, Germany — <sup>6</sup>KTH Royal Institute of Technology, Teknikringen 56-58, 100 44 Stockholm, Sweden

Poly(3-hexylthiophen-2,5-diyl) (P3HT) is one of the most prominent semiconducting, conjugated polymers in the fields of organic electronics and photovoltaics. Upon addition of a suitable metal dopant, e.g. chloroauric acid (HAuCl<sub>4</sub>), thin P3HT films exhibit thermoelectric properties with large values for the power factor and figure of merit. To investigate the possibility and efficiency of future scalable industrial manufacturing, spin-casted and spray-deposited P3HT films were compared correlating their structural differences with their thermoelectric performance upon doping using AFM, GISAXS/GIWAXS, XRR and NR measurements.

CPP 27.3 Wed 12:00 H39

**In-situ GISAXS Observation and Large Area Homogeneity Study of Slot-Die Printed PS-b-P4VP and PS-b-P4VP/FeCl<sub>3</sub> Thin Films** — ●SHANSHAN YIN<sup>1</sup>, TING TIAN<sup>1</sup>, CHRISTIAN L. WEINDL<sup>1</sup>, KERSTIN S. WIENHOLD<sup>1</sup>, QING JI<sup>2</sup>, YAJUN CHENG<sup>2</sup>, YANAN LI<sup>3</sup>, CHRISTINE M. PAPADAKIS<sup>3</sup>, MATTHIAS SCHWARTZKOPF<sup>4</sup>, STEPHAN V. ROTH<sup>4,5</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,6</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — <sup>2</sup>NIMTE, Chinese Academy of Sciences, 315201, P. R. China — <sup>3</sup>TU München, Physik-Department, Fachgebiet Physik weicher Materie, 85748 Garching — <sup>4</sup>DESY, 22607 Hamburg — <sup>5</sup>Royal Institute of Technology KTH, 100 44 Stockholm — <sup>6</sup>MLZ, TU München, 85748 Garching

Mesoporous hematite (Fe<sub>2</sub>O<sub>3</sub>) thin films with high surface-to-volume ratios show great potential as photoelectrodes or electrochemical electrodes in energy conversion and storage. In the present work, with the assistance of an up-scalable slot-die coating technique, highly ordered Fe<sub>2</sub>O<sub>3</sub> thin films are successfully printed based on the amphiphilic diblock copolymer poly(styrene-*b*-4-vinyl pyridine) (PS-*b*-P4VP) as a

structure-directing agent. Pure PS-*b*-P4VP films are printed under the same conditions for comparison. The micellization of the diblock copolymer in the solution, the film formation process of the printed thin films, the homogeneity of the dry films in the lateral and vertical direction as well as the morphological and compositional information of the calcined hybrid PS-*b*-P4VP/FeCl<sub>3</sub> thin film are investigated.

CPP 27.4 Wed 12:15 H39

**Morphology transformation pathway of block copolymer-directed cooperative self-assembly of ZnO hybrid films monitored in situ during slot-die coating** — ●TING TIAN<sup>1</sup>, SHANSHAN YIN<sup>1</sup>, SUO TU<sup>1</sup>, CHRISTIAN L. WEINDL<sup>1</sup>, KERSTIN S. WIENHOLD<sup>1</sup>, SUZHE LIANG<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, STEPHAN V. ROTH<sup>2,3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,4</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — <sup>2</sup>DESY, 22607 Hamburg — <sup>3</sup>KTH, Department of Fibre and Polymer Technology, 10044 Stockholm, Sweden — <sup>4</sup>MLZ, TU München, 85748 Garching

Co-assembly of diblock copolymers (DBC) and inorganic precursors that takes inspiration from the rich phase separation behavior of DBCs can enable the realization of a broad spectrum of functional nanostructures with the desired sizes. In a DBC assisted sol-gel chemistry approach with polystyrene-block-poly(ethylene oxide) and ZnO, hybrid films are formed with slot-die coating. In situ GISAXS measurements are performed to investigate the self-assembly and co-assembly process during the film formation. Combining complementary ex situ characterizations, several distinct regimes are differentiated to describe the morphological transformations from the solvent-dispersed to solidified films. The comparison of the assembly pathway evidences that the key step in the establishment of the pure DBC film is the coalescence of spherical micelles toward cylindrical domains. Due to the presence of the precursor, the formation of cylindrical aggregates in the solution is crucial for the structural development of the hybrid film.

CPP 27.5 Wed 12:30 H39

**Programmable Luminescent Tags: Utilizing the interplay of room temperature phosphorescence and oxygen as an information storage device** — ●TIM ACHENBACH, MAX GMELCH, HEIDI THOMAS, and SEBASTIAN REINEKE — Technische Universität Dresden, Germany

By utilizing the interaction between molecular oxygen and the room temperature phosphorescence of organic materials, continuous-wave-readable and sub-second programmable luminescent tags (PLT) can be realized. They are transparent, flexible and provide a resolution of up to 700 dpi. Information is imprinted by illuminating the PLT with UV light through a shadow mask. By heating the PLT, the information can be erased and a new writing cycle can be started again.

The device consists of two layers on a substrate. The functional layer comprises an organic biluminescent emitter doped into a polymer. The second layer is an oxygen barrier layer. After wet processing in air, molecular oxygen is present in the functional layer of the device, quenching the phosphorescence of the emitter. As energy is transferred to the oxygen during this interaction, it is excited to its highly reactive singlet state and binds to its environment. Over time, all molecular oxygen in the illuminated areas undergoes this photo-consumption process, and a phosphorescent pattern in shape of the mask becomes visible. The oxygen barrier becomes more permeable at elevated temperatures, allowing an oxygen refill of the functional layer by heating the device. This resets the device and it can be rewritten after a short cooling phase.

CPP 27.6 Wed 12:45 H39

**Spatio-temporal Imaging of Programmable Luminescent Tags reveals Planar Oxygen Diffusion Properties in Polymer Films** — ●RICHARD KANTTELBERG, TIM ACHENBACH, ANTON KIRCH, and SEBASTIAN REINEKE — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Germany

Programmable Luminescent Tags based on oxygen quenched organic room temperature phosphorescence show application potential in UV sensing and re-writable labelling. This work demonstrates, that the concept can also be exploited to resolve oxygen diffusion properties in

thin polymer films, which are essential in everyday applications from medical encapsulation to industrial packaging. In contrast to many established methods, the investigated principle comes without the need of complex pressure sensitive setups or vacuum technology and potentially allows high spatial accuracy. The time-resolved tracking of

a two-dimensional phosphorescent pattern reveals the in-plane oxygen diffusion coefficient and considers the photoconsumption of oxygen during the measurement. The diffusion coefficients are determined at the representative case of polystyrene glasses with molecular weights between 13 000 and 350 000 g/mol.