

## HL 17: Organic Semiconductors

Time: Tuesday 9:30–12:00

Location: EW 015

HL 17.1 Tue 9:30 EW 015

**Charge mobility in polar columnar phases of subphthalocyanine containing liquid crystals** — ●AHMAD MURAD<sup>1</sup>, ELIAS BARON<sup>1</sup>, MARTIN FENEBERG<sup>1</sup>, MAXIMILIAN BAUMANN<sup>2</sup>, MATTHIAS LEHMANN<sup>2</sup>, and ALEXEY EREMIN<sup>1</sup> — <sup>1</sup>Otto-von-guericke-Universität — <sup>2</sup>Julius-Maximilians-Universität Würzburg

We report measurements of time-of-flight charge carrier mobility in star-shaped mesogens with subphthalocyanine core that forms self-assembled polar columnar phases. The study investigates the intricate interplay between temperature and electric field dependence on the high mobility of polar columnar phase liquid crystals (PCLCs). We demonstrate that the charge mobility exhibits an anomalous field dependence decreasing with increasing electric field. PCLCs exhibit unique structural properties characterized by self-assembled columnar arrangements of mesogens with spontaneous polarisation, which make them promising candidates for various electronic and optoelectronic applications.

HL 17.2 Tue 9:45 EW 015

**Optical and electrically driven single-molecular Raman switch** — ●HAI BI — Jihua Laboratory, No.28 Huandao South road, Nanhai district, Foshan 528200, China

We have presented a single-molecular Raman switch, which is controlled not only by an applied voltage, but also by optical inputs with different directions. In this study, the combined effect of the near-field optical angular momentum and the bias voltage on the Raman response of a single molecular junction, creating a molecular switch, was investigated. It was demonstrated that the molecular switch can be manipulated using an optical input. The effects of both the polarisation of light and the subsequent symmetry properties of the electromagnetic near field were investigated and used to control the switching behaviour. This change in the Raman response of the junction is associated with a modification of the conformation of the molecule. By changing both the illumination side and the voltage applied to the junction, the Raman intensity can be turned ON and OFF with a difference of nearly five orders of magnitude between the two states.

HL 17.3 Tue 10:00 EW 015

**Isotope effects in Ga- and O-rich monoclinic  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>** — ●DANIEL CIERPINSKY<sup>1</sup>, BENJAMIN M. JANZEN<sup>1</sup>, ANDREA ARDENGHI<sup>2</sup>, OLIVER BIERWAGEN<sup>2</sup>, PIERO MAZZOLINI<sup>3</sup>, ROLAND GILLEN<sup>4</sup>, JANINA MAULTZSCH<sup>4</sup>, ANDREAS FALKENSTEIN<sup>5</sup>, JOE KLER<sup>5</sup>, ROGER SOUZA<sup>5</sup>, MANFRED MARTIN<sup>5</sup>, and MARKUS R. WAGNER<sup>2,1</sup> — <sup>1</sup>Technische Universität Berlin, Germany — <sup>2</sup>Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — <sup>3</sup>University of Parma, Italy — <sup>4</sup>Chair of Experimental Physics, Erlangen, Germany — <sup>5</sup>RWTH Aachen University, Aachen, Germany

We employ polarization-dependent confocal micro-Raman spectroscopy to study the vibrational properties of isotopic  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. For this purpose samples were fabricated using molecular beam homoepitaxy to produce thin films of <sup>18</sup>O isotopic Ga<sub>2</sub>O<sub>3</sub> on non isotopic <sup>16</sup>O Ga<sub>2</sub>O<sub>3</sub> substrate, with growth conditions ranging from metal- to oxygen-rich regimes. We determine the spectral position of all Raman active phonon modes with high precision and observe that the substitution of <sup>16</sup>O with <sup>18</sup>O leads to shifts towards lower frequencies for all modes due to the higher isotopic mass. The isotopically induced shifts and their variations resulting from different growth regimes are discussed in conjunction with DFT calculations on the phonon energy contribution of lattice sites as well as SIMS measurements.

HL 17.4 Tue 10:15 EW 015

**Excitons in organic materials: Revisiting old concepts with new insights** — ●S. ANHÄUSER<sup>1</sup>, D. BISCHOF<sup>1</sup>, A.M. VALENCIA<sup>2</sup>, C. COCCHI<sup>2</sup>, and G. WITTE<sup>1</sup> — <sup>1</sup>Philipps-Universität Marburg, FB Physik — <sup>2</sup>Carl von Ossietzky Universität Oldenburg, FB Physik

The concept of excitons, originally developed for inorganic materials, is often directly transferred to organic materials, ignoring key differences in the properties of their optical excitations. Here we report a combined experiment/theory study carried out for acenes with focus on tetracene and perfluorotetracene, in order to critically examine these concepts. For this purpose we combine detailed optical spectroscopy of various states of matter ranging from solution, to poly- and single

crystalline samples, and even melt, with state-of-the-art first-principles calculations, based on DFT and many-body methods on top. This integrated approach provides deep insights into the optical signatures of the organic systems and enables us to distinguish the single particle nature of excitations in isolated molecules from the collective nature of excitons in all aggregated phases. This shows that quantum mechanical interactions between similar molecules represent a critical link between these two scenarios [1]. Therefore, we propose to use the term 'exciton' only for optical excitations of aggregated molecular materials. The presented results not only provide a deeper understanding of the optical excitations in organic semiconductors, but also highlight roadmaps and potential pitfalls that need to be considered when studying these systems.

[1] A.M. Valencia et al., Electron. Struct. 2023, 5, 033003.

HL 17.5 Tue 10:30 EW 015

**Thermal Stability of Doped Organic Hole Transport Layers** — ●STEPHANIE BUCHHOLTZ, TOBIAS ANTRACK, HANS KLEEMANN, and KARL LEO — Dresden Integrated Center for Applied Physics and Photonic Materials, Dresden, Germany

The electrical conductivity of amorphous doped organic hole transport layers, as used in organic light-emitting diodes (OLEDs), solar cells or photodetectors, increases with temperature due to the dominant hopping-like transport mechanism. However, the conductivity breaks down irreversibly at a certain temperature. For example, OLEDs and organic photovoltaics have operating temperatures up to 80°C and 145°C, respectively. In addition, the active layer of an organic solar cell is deposited on the hole transport layer and has to be annealed at temperatures up to 140°C for a higher efficiency. The cause of the breakdown is unknown, which impedes the development of more stable devices. Here we show a relation between the breakdown of the conductivity and the glass transition of the small molecule host materials and find that the choice of the dopant and the doping concentration significantly affect the thermal stability of the layer. Based on our investigations, we develop different hypotheses about the cause of the breakdown. With our results, we devised strategies to improve the thermal stability of organic hole transport layers.

15 min. break

HL 17.6 Tue 11:00 EW 015

**Room-temperature polariton lasing and photonic confinement in an organic microcavity** — ●DOMINIK HORNEBER<sup>1</sup>, JOHANNES DÜRETH<sup>1</sup>, TIM SCHEMBRI<sup>2</sup>, SIMON BETZOLD<sup>1</sup>, SVEN HÖFLING<sup>1</sup>, MATTHIAS STOLTE<sup>2</sup>, FRANK WÜRTHNER<sup>2</sup>, and SEBASTIAN KLEMBT<sup>1</sup> — <sup>1</sup>Julius-Maximilians-Universität Würzburg, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Lehrstuhl für Technische Physik, Am Hubland, 97074 Würzburg, Deutschland — <sup>2</sup>Center for Nanosystems Chemistry (CNC), Julius-Maximilians-Universität Würzburg, Theodor-Boveri-Weg, 97074, Würzburg, Deutschland

Perylene bisimides (PBIs) are organic dyes with quantum yields (PLQY) close to unity and excellent thermal and photo-chemical stability. These features as well as the tunability of their solid-state packing via chemical functionalization make this material class a promising candidate for lasing at room temperature. In this work, we show strong light-matter interaction and exciton-polariton lasing in optical microcavities with a neat layer of a PBI monomer that is shielded by voluminous bay-substituents to prevent aggregation-induced PLQY-quenching. Furthermore, photonic confinement in zero-dimensional resonators and chains of coupled resonators is demonstrated which shows the energetic discretization of the modes and the formation of a band-structure, respectively. This paves the way for the study of non-linear bosonic systems in artificial lattices hosting a highly stable PBI as solid-state emitter.

HL 17.7 Tue 11:15 EW 015

**Interplay of Electrical Conductivity and Seebeck Coefficient of n-doped NDI-based Polymer Thin Films for Thermoelectric Applications** — ●MARIE SIEGERT<sup>1</sup>, MARKUS HÖNIG<sup>2</sup>, MICHAEL SOMMER<sup>2</sup>, and JENS PFLAUM<sup>1,3</sup> — <sup>1</sup>University of Würzburg — <sup>2</sup>Chemnitz University of Technology — <sup>3</sup>CAE Bayern

Thermoelectric generators based on organic materials offer a sustainable, low-cost approach towards waste heat recovery and thus, efficient energy consumption. Disordered polymer thin films in particular exhibit aptly low thermal conductivities  $\kappa$  for thermoelectric applications and their preparation via solution processing is easily scaled to meet industrial requirements. To improve their inherently low charge carrier concentration and therefore increase their electrical conductivity  $\sigma$ , suitable dopants can be employed. However, doping typically causes the Seebeck coefficient  $S$  to decrease, and may even lead to a polarity change in  $S$  at high doping concentrations, which is detrimental to thermoelectric efficiency. Here we conducted temperature dependent studies on thin films of the polymer PNDIT2 utilizing the n-type dopant TAM with regards to their thermoelectric properties. Systematically varying the molecular weight of the PNDIT2 host, the interplay of charge carrier density and mobility in this polymeric system and their effect on the Seebeck coefficient are revealed. The resulting power factors  $PF = \sigma S^2$  suggest future strategies to further refine the doping protocol for polymer thin films and thus, to maximize their thermoelectric figure of merit. The Deutsche Bundesstiftung Umwelt (DBU) is acknowledged for financial support.

HL 17.8 Tue 11:30 EW 015

**Polymer-Metal-Composite Films with Structural Anisotropy for Thermoelectric Applications** — •CHRISTIAN GRADL<sup>1</sup>, MARIE SIEGERT<sup>1</sup>, and JENS PFLAUM<sup>1,2</sup> — <sup>1</sup>Julius-Maximilians-Universität Würzburg, 97074 Würzburg — <sup>2</sup>CAE Bayern, 97074 Würzburg

To address the intrinsic limitations of neat organic semiconductors in thermoelectric (TE) applications, the fabrication of composites offers a promising approach by synergizing the best properties of the individual components. Inducing spatial order within such composite films can further enhance their TE performance. We applied this concept to the crystalline 1D molecular p-type metal TTT<sub>2</sub>I<sub>3</sub> which has intriguing potential for TE applications due to its high electrical and low thermal conductivity. Our research focuses on exploiting these TE properties in conjunction with the anisotropic spatial orientation of the microcrystals within PEDOT:PSS polymer films. The TTT<sub>2</sub>I<sub>3</sub>

crystals are grown by microspacing in-air sublimation on single crystal RbCl substrates under ambient conditions. The self-alignment of the microcrystals originates from the growth on the respective RbCl surface facet and, hence, can be modified by the specific choice of a certain surface orientation. Subsequently, the aligned TTT<sub>2</sub>I<sub>3</sub> microcrystals were enclosed by a solution processed p-type conducting PEDOT:PSS layer to finalize the composite thin film preparation. By the analysis of the thermoelectric properties, we are able to highlight the role of the 1D organic metal additives and their anisotropic spatial alignment on the TE characteristics of the polymer-metal composite films.

HL 17.9 Tue 11:45 EW 015

**Direct observation of the energy band structure of the super atom molecular orbital in solid phase C60** — •DAICHI HOMMA<sup>1</sup>, SUSUMU YANAGISAWA<sup>2</sup>, and HIROYUKI YOSHIDA<sup>1,3</sup> — <sup>1</sup>Graduate School of Engineering, Chiba University, Chiba, Japan — <sup>2</sup>Faculty of Science, University of the Ryukyus, Okinawa, Japan — <sup>3</sup>Chiba University MCRC, Chiba, Japan

The Super Atom Molecular Orbital (SAMO) is a hydrogen-like unoccupied orbital in which an electron is loosely bound around a central Coulomb potential of a molecule. Because of this nature, SAMO is predicted to form nearly free electron (NFE) bands in solids, which should exhibit high electron mobility. SAMO was first observed in C60 [1] and has so far only been observed in the monolayer and in the gas phase. To discuss the electron mobility in the solid phase, it is essential to detect the SAMO and measure the band structure in the solid state.

Recently, we have developed angle-resolved low-energy inverse photoelectron spectroscopy [2]. Using this technique, we observed the s-SAMO of C60 in bulk for the first time and further revealed the band structure. We prepared a 10 nm thick epitaxially grown C60 film on the Cu(111). From the comparison with the previous studies, we assigned a peak 2.97eV above the LUMO band as the SAMO-derived band. The observed band structure is NFE-like with an effective mass of 1.35  $m_e$ . [1] M. Feng, et al., Science 320, 359 (2008). [2] Y. Kashimoto, et al., Rev. Sci. Instrum. 94, 063903 (2023).