# CPP 29: Organic Electronics and Photovoltaics III

Time: Wednesday 15:00–16:00 Location: H38

CPP 29.1 Wed 15:00 H38

**Energy band structure of image potential states of organic semiconductor on graphite studied by angle-resolved low-energy inverse photoelectron spectroscopy** — •Tomoko Onishi[1] and Hiroyuki Yoshida[1,2] — [1]Chiba university, Chiba, Japan. — [2]Chiba university MCRC, Chiba, Japan.

The image potential state of the organic semiconductor molecule on the conductive surface is of particular interest because the image potential states can be sensitive probes of interfacial electronic states. Their energy band structure (the energy-momentum relation) provides detailed information about the electron behavior. Recently, we have developed the angle-resolved low-energy inverse photoelectron spectroscopy (AR-LEIPS) [1,2]. This technique allows direct observation of the unoccupied states without sample damage and with the resolution better than 0.3 eV. In this study, we applied AR-LEIPS to a monolayer of copper phthalocyanine (CuPc) on highly oriented pyrolytic graphite (HOPG). The observed band structure of the image potential state was parabolic, indicating that its nature is free-electron-like along the surface plane. By fitting the band structure to a quadratic function, we obtained the effective masses of the image potential states on HOPG and CuPc/HOPG to be (1.14 * 0.02) m0 and (1.33 * 0.08) m0, respectively, where m_0 is the electron mass. The effective mass becomes heavier due to the periodic potential induced by the CuPc molecule.[1] H. Sato, H. Ishii, H. Yoshida, et al., Nature Mat. 21, 916 (2022) [2] Y. Kashimoto, H. Yoshida et al, Rev. Sci. Instrum., 94, 063903 (2023).

CPP 29.2 Wed 15:15 H38

**Fluorination of Thieno-quinoxalines enables tunable excitonic and electronic bandgaps** — •Md Moidul Islam[1,2], Arthur Markus Anton[3], Shahidul Alam[4], Patrick Irmisch[3], Alexander J. Much[7], Ulrich S. Schubert[1,2], Christos Chochos[5,6], and Harald Hoppe[1,2] — [1]IOMC, FSU Jena, Humboldtstrasse 10, 07743 Jena, Germany — [2]CEEC Jena, Philosophenweg 7a, 07743 Jena, Germany — [3]Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig — [4]KAUST Solar Center, PSE, MSE, Thuwal 23955-6900, Kingdom of Saudi Arabia — [5]Institute of Chemical Biology, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 11635, Greece — [6]Advent Technologies SA, Patras Science Park, Stadiou Street, Platani-Rio, 26504, Patra, Greece — [7]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Thieno-quinoxaline conjugated polymers are an interesting class of organic semiconductors. While it is known that fluorination causes shifts in the molecular energy levels to deeper binding energies, the mechanisms behind are, so far, not well characterized. In this study, six thieno-quinoxaline polymers with a systematically increased number of fluorinated sites were investigated in solutions and films. Our results indicate a strong correlation between the extend of fluorination, the molecular planarity, and its ability to form aggregates. We also demonstrate, in unprecedented detail, how these structural properties influence various behaviors related to optical and electronic properties.

CPP 29.3 Wed 15:30 H38

**Extending the design space of carbazole-based TADF emitters: From photophysical insights to OLED performance** — •Karolis Leitonas[1], Łukasz Łapok[2], Sebastian Schellhammer[1], and Sebastian Reineke[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden — [2]Department of Physical Chemistry and Electrochemistry, Faculty of Chemistry, Jagiellonian University, Kraków, Poland

Although organic light-emitting diodes (OLEDs) dominate the market for mobile displays, e.g., in smartphones, designing efficient and long-lasting blue pixels remains challenging. Enhancing OLED efficiency requires effective singlet and triplet exciton harvesting - a key mechanism to minimize energy losses via non-radiative decay. Emitter materials exhibiting thermally activated delayed fluorescence (TADF) can achieve up to 100 % internal quantum efficiency (IQE) providing a promising approach for the design of efficient OLEDs. Still, their potential is not yet fully exploited due to incomplete insights into the underlying structure-property relationships and chemical design challenges. We discuss the photophysical properties of new emitters extending the class of carbazole-based TADF emitters introduced by Adachi et al. [1] and analyze their application in OLEDs.

[1] Uoyama et al. Nature 2012

CPP 29.4 Wed 15:45 H38

**Predicting the molecular arrangement of organic optoelectronic materials** — •Alexey Gudovannyy[1], Julia M. Schäfer[2], Olga Gerdes[2], Dirk Hildebrandt[2], Gunter Mattersteig[2], Martin Pfeiffer[2], and Frank Ortmann[1] — [1]Department of Chemistry, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [2]Heliatek GmbH, 01139 Dresden, Germany

The morphology of the most promising molecular semiconductor materials remains highly challenging to predict from scratch. If possible, it would still require a lot of computational time and sometimes experimental data. The main obstacle here is the exponential growth with the number of molecular degrees of freedom for bulky side groups, which forces one to search on extremely complex energy surfaces. However, organic semiconductors mostly exhibit a limited set of structural motifs, primarily herringbone and two-dimensional brickwork patterns. Constraining the search to such dimensionally reduced packing possibilities simplifies the process while preserving 3D structural features. Here, we present a cost-efficient workflow for predicting thermodynamically stable 2D arrangements of molecular periodic associates, where only the molecular structural formula is required. We theoretically and experimentally investigated a set of known and newly crystallized compounds of evaporable flexible molecules with interesting optoelectronic properties, predicted their packing in two-dimensional layers, and compared them with experimentally resolved crystal structures, obtaining a very good agreement in the packing.