

CPP 5: Poster Session I

Electrical, Dielectrical and Optical Properties of Thin Films (1-7); Hybrid and Perovskite Photovoltaics (8-13); Organic Electronics and Photovoltaics (14-16); Molecular Electronics and Excited State Properties (17-19).

Time: Tuesday 17:30–19:30

Location: P

CPP 5.1 Tue 17:30 P

Thermal degradation of EMIM DCA post-treated PEDOT:PSS thermoelectric thin films, investigated via in-situ GISAXS — ●ANNA LENA OECHSLE¹, JULIAN E. HEGER¹, NIAN LI¹, SHANSHAN YIN¹, SIGRID BERNSTORFF², and PETER MÜLLER-BUSCHBAUM^{1,3} — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²ELETTRA Sincrotrone Trieste S. C. p. A., 34149 Basovizza TS, Italy — ³Heinz Maier-Leibnitz Zentrum (MLZ), TU München, 85748 Garching, Germany

The constantly increasing energy demand raises the need for renewable energies and the reduction of energy dissipation. Thermoelectric materials are promising in terms of waste heat recovery and the use of solar thermal energy, as they enable the direct conversion of a temperature gradient into electrical power. Nowadays great research focus is especially on thermoelectric polymers, as they are low or nontoxic, lightweight, flexible and allow a low-cost, large-scale solution-based production of thin films. In this work we show the positive influence of EMIM DCA post-treatment on the Seebeck coefficient and electrical conductivity of PEDOT:PSS thin films. However, for possible future applications it is also important to understand the behavior of these films during long-term operation at elevated temperature. Therefore, we reveal occurring morphology changes with in-situ GISAXS measurements of these films and try to link them to the observed decrease in the electrical conductivity.

CPP 5.2 Tue 17:30 P

Uncovering the enhancement mechanisms of thermoelectric performance of PEDOT: PSS films after physical-chemical dedoping — ●SUO TU, TING TIAN, ANNA-LENA OECHSLE, and PETER MÜLLER-BUSCHBAUM — Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

Organic semiconductors have attracted intense attention because of their potential use in mechanically flexible, lightweight, and inexpensive electronic devices. Especially* PEDOT: PSS is the most studied conducting polymer system due to their intrinsically high electrical conductivity, low thermal conductivity, and high mechanical flexibility in thermoelectric (TE) devices. It is generally acknowledged that it is difficult to achieve a high ZT value of TE materials, due to the fact that the interdependence of parameters as a function of charge carrier concentration. In this work, we adopt a combination of DMSO addition and subsequent DMSO/salt mixture post-treatment to improve the TE performance of PEDOT: PSS thin films. Results show that the as-obtained PEDOT: PSS film presents a maximum PF of 105.2 *W(m-1K-2), which is ~1750-fold leap larger than that of pristine film. The origin and mechanism of the underlying improvement are systematically investigated by various characterizations to gain a more profound understanding of the fundamental nature of the modified PEDOT: PSS films.

CPP 5.3 Tue 17:30 P

Measurement setup to characterize thermoelectric polymer thin films — ●SIMON WEGENER¹, ANNA LENA OECHSLE¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The growing need to save fossil resources requires, besides their substitution, also their effective usage. This usage is mostly limited by the high amounts of wasted heat in the conversion from chemical energy to mechanical or electrical energy. Thermoelectric (TE) materials are a promising way to make use of this wasted energy. Particularly, they can be used in a wide range of applications to generate electricity. Nevertheless, these materials show lots of room for improvement in terms of their output power. Therefore, with our work, we aim to construct a setup, which focuses especially on the measurement of polymer-based TE materials for low-temperature applications. This setup consists

of two mounting plates that can be heated or cooled individually to determine the Seebeck coefficient. Additionally, a van der Pauw measurement can be done to find the electrical conductivity of the sample. By this, the setup will enable the user to rapidly characterize samples by its TE power factor.

CPP 5.4 Tue 17:30 P

Tailoring the Optical Properties of Sputter-Deposited Gold Nanostructures on Nanostructured Titanium Dioxide Templates — ●SUZHE LIANG¹, WEI CHEN¹, SHANSHAN YIN¹, SIMON J. SCHAPER¹, JONAS DREWES², NIKO CARSTENS², THOMAS STRUNSKUS², FRANZ FAUPEL², MARC GENSCHE^{1,3}, MATTHIAS SCHWARTZKOPF³, STENPHAN V. ROTH^{3,4}, and PETER MÜLLER-BUSCHBAUM^{1,5} — ¹TU München, Garching, Germany — ²CAU, Kiel, Germany — ³DESY, Hamburg, Germany — ⁴KTH, Stockholm, Sweden — ⁵MLZ, TU München, Garching, Germany

Au/TiO₂ nanohybrid materials have attracted significant attention due to the outstanding optical, photocatalytic and photovoltaic performance. We use customized polymer templating to achieve TiO₂ nanostructures with different morphologies. Au/TiO₂ hybrid thin films are fabricated by sputter deposition. An in-depth understanding of the Au morphology on the TiO₂ templates is achieved with in situ GISAXS during the sputter deposition. The resulting Au nanostructure is largely influenced by the TiO₂ template morphology. Based on the detailed understanding of the Au growth process, characteristic distances can be selected to achieve tailored Au nanostructures at different Au loadings. For selected sputter-deposited Au/TiO₂ hybrid thin films, the optical response with a tailored localized surface plasmon resonance is demonstrated.

CPP 5.5 Tue 17:30 P

Sputter-deposition vs. spraying: effect of doping technique on the structural and thermoelectric properties of P3HT-based thin films — ●BENEDIKT SOCHOR¹, CONSTANTIN HARDER¹, ANNA-LENA OECHSLE², MATTHIAS SCHWARTZKOPF¹, ALEXEI VOROBIEV³, PETER MÜLLER-BUSCHBAUM², and STEPHAN V. ROTH^{1,4} — ¹Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — ²Technical University Munich, Physics Department, James-Franck-Str. 1, 85748 Garching, Germany — ³Institut Laue-Langevin, 71 Avenue des Martyrs, 38042 Grenoble Cedex 9, France — ⁴KTH 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. This study aims for correlating process and fabrication parameters and the structural changes with the overall thermoelectric performance of P3HT and P3HT:PMMA films. Especially, we focus on two routes of gold (Au) doping, namely sputter and spray deposition techniques. The structure of the resulting polymer composites indicated distinct differences whether the gold is sprayed or grown on the surface as shown by AFM as well as neutrons and X-ray reflectivity measurements. During in situ GISAXS experiments, the growth and structure of the gold particles was mapped, which indicated the presence of sub-nanometer sized gold clusters in case of sputter deposition.

CPP 5.6 Tue 17:30 P

Hybrid energy harvester based on triboelectric nanogenerator and solar cell — ●TIANXIAO XIAO¹, WEI CHEN¹, WEI CAO¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — ²Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße. 1, 85748 Garching, Germany

Developing clean energy lies the heart of sustainable development of human society. Triboelectric nanogenerator (TENG) originating from Maxwell's displacement current is a new type of energy harvester for harnessing ambient mechanical energy based on the coupling of tribo-

electrification and electrostatic induction effect. Compared with other counterparts, owing to the light-weight, low-cost, and easily fabricated, TENG has become one of the most promising candidates in replacement of conventional fossil fuels and attracted worldwide attention in the past years. However, to further increase the energy harvesting efficiency and broaden application fields, integrating the TENG with other kinds of energy harvesters in one device is a possible way to meet these needs. In the present work, a TENG based hybrid energy harvester is designed and fabricated on the flexible polyethylene terephthalate (PET) substrate. This hybrid device consists of a single-electrode mode TENG component and a PbS quantum dots based solar cell component, which can harness both mechanical and solar energy from ambient environment to directly generate electricity.

CPP 5.7 Tue 17:30 P

Colloidal photonic crystal slabs toward enhanced photoconductivity — ●SWAGATO SARKAR¹, VAIBHAV GUPTA², and TOBIAS A. F. KÖNIG^{1,3} — ¹Leibniz-Institut für Polymerforschung Dresden e.V. (IPF), Institute for Physical Chemistry and Polymer Physics, Hohe Str. 6, 01069 Dresden, Germany — ²Institute of Particle Technology, Friedrich-Alexander University Erlangen-Nürnberg, Cauerstrasse 4, 91058 Erlangen, Germany — ³Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden 01062 Dresden, Germany

In the present work, a fusion of interference lithography (IL) and nanosphere imprint lithography [Gupta, König, Fery, ACS Appl. Mater. Interfaces 2019, 11, 28189.] on various target substrates ranging from carbon film on transmission electron microscope grid to inorganic and dopable polymer semiconductor is reported. 1D colloidal photonic crystals are printed with 75% yield on the centimeter scale using colloidal ink and an IL-produced polydimethylsiloxane stamp. Atomically smooth facet, single-crystalline, and monodisperse colloidal building blocks of gold (Au) nanoparticles can produce 1D plasmonic grating on top of a titanium dioxide (TiO₂) slab waveguide, producing waveguide-plasmon polariton [Sarkar, Fery, König, Adv. Funct. Mater. 2021, 31, 2011099.] modes with superior 10 nm spectral line-width. Plasmon-induced hot electrons are confirmed via two-terminal current measurements resulting in increased photoresponsivity as well as enhanced photocatalytic degradation of methyl orange (MO) dye molecules.

CPP 5.8 Tue 17:30 P

Upscaling Perovskite: Optoelectronics and Morphology of Slot-Die Coated Solar cells — ●ANDREA VITALONI¹, LENNART K. REB¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — ²Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite solar cells (PSCs) have attracted increasing attention in research and industry due to their high efficiency, low material cost, and simple solution-based fabrication process. Additionally, the possibility to fabricate flexible and thin solar cells creates new opportunities compared to traditional solar modules.

In laboratory devices, the efficiency already exceeds 25% and is comparable with c-Si. However, one of the most important steps towards commercialization is the upscaling of the PSCs production to larger areas. Slot-die coating is considered to be one of the most promising technology, being a fast process with minimum material consumption and waste. Furthermore, the highly tuneable perovskite ink composition strongly determines kinetic processes during film formation and the final morphology.

We vary the composition of MAPI inks and analyze the printed perovskite thin-films and derived solar cells with spectroscopic and X-ray scattering methods. The focus is on developing a comprehensive understanding of the slot-die coating process for printed, flexible, and high-efficiency PSCs.

CPP 5.9 Tue 17:30 P

In-Operando study of humidity on the performance of perovskite solar cell — ●KUN SUN¹ and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — ²Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite solar cells (PSCs) are one of the most promising photo-

voltaic technologies and reached a certified 25.2% efficiency owing to their tuneable bandgap, high carrier mobility, long diffusion length and so on. The long-term operational stability of PSCs, however, has been not investigated. Herein, we probe the structure change with grazing-incidence small-angle scattering (GISAXS) under high humidity. Also, the solar cell parameters are obtained simultaneously during the device operation. We find that PSCs fabricated with and without caesium iodide (CsI) show differences in the device degradation and morphology change in the perovskite layer. The decrease of open-circuit voltage (VOC) can be attributed to the morphology changes and the evolution of crystallize grain size. With the additive of CsI, solar cells show slow decay of VOC, which is correlated to improved morphology of active layer and passivation of trap states. Our work presents a crucial step towards a fundamental understanding of morphology change combined with solar cell parameters during the device operation.

CPP 5.10 Tue 17:30 P

Tailoring the orientation of perovskite crystals via adding two-dimensional polymorphs for perovskite solar cells — ●RENJUN GUO¹, ALI BUYRUK², XINYU JIANG¹, WEI CHEN¹, LENNART K. REB¹, MANUEL A. SCHEEL¹, TAYEBEH AMERI², and PETER MÜLLER-BUSCHBAUM¹ — ¹Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany — ²Chemie-Department, Ludwig-Maximilians-Universität München, Butenandtstr. 5-13 (E), 81377 München, Germany

Due to their outstanding properties, organic-inorganic perovskite materials are gaining increasing attention for their use in high-performance solar cells. Finding an effective method of defect passivation is thought to be a promising path for advancements toward narrowing the distribution of the power conversion efficiency (PCE) values, as measured by the spread in the PCE over different devices fabricated under identical conditions, for easier commercialization. We add 2*(4*fluoroph-enyl)ethyl ammonium iodide (p-f-PEAI) into the bulk of a mixed cation lead halide perovskite film in this study. The addition of the appropriate amount of p-f-PEAI affects the preference orientation of the perovskite crystals, increases the strength of the crystal texturing, and reduces non-radiative charge recombination. As a result, we achieve a tighter range of the PCE of perovskite solar cells (PSCs) without losing the PCE values obtained [1].

[1] Guo et al. J. Phys. Energy 2, 034005 (2020)

CPP 5.11 Tue 17:30 P

Fabrication and characterisation of slot-die coated formamidinium-cesium lead iodide perovskite solar cells — ●ALEXANDER FRANZ WEINZIERL¹, MANUEL A. SCHEEL¹, LENNART K. REB¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — ²Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite solar cells (PSC) are a promising candidate to evolve the solar energy market due to high energy conversion efficiencies and low cost material usage. However, many perovskite absorber compositions suffer from long-term stability problems. Perovskites, composited of formamidinium/caesium lead iodide/bromide (FACs), as the active layer of such solar cells are promising to overcome this issue. Crucial for FACs is the development of a solvent system together with an optimised printing process enabling to produce highly homogeneous layers and, as a result, cells with high performance and low degradation. To achieve this outcome, slot-die coating is examined for depositing the Perovskite ink, especially, since this printing technique is transferable to the scale-up of PSCs towards commercial sizes. In this work inverted slot-die coated FACs solar cells are produced with different solvents. Their film morphology is investigated by microscopy, X-ray diffraction and GIWAXS. Moreover, the cells are characterised and compared via their respective current-voltage characteristic, giving insight into the performance parameters.

CPP 5.12 Tue 17:30 P

The Influence of CsBr on Crystal Orientation and Optoelectronic Properties of MAPbI₃-based Solar Cells — ●YUQIN ZOU and PETER MÜLLER-BUSCHBAUM — Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany.

Crystal orientations are closely related to the behavior of the photo-generated charge carrier and vital for controlling the optoelectronic properties of perovskite solar cells. Herein, we propose a facile ap-

proach to reveal the effect of lattice plane orientations on the charge carrier kinetics via constructing CsBr doped mixed-cation perovskite phases. Through GIWAXS measurements, we systematically investigate the crystallographic properties of mixed perovskite films in the microscopic scales and reveal the effect of the extrinsic CsBr doping on the stacking behavior of the lattice planes. And provides a unique insight into the underlying relationship among the stacking pattern of crystal planes, the photo-generated charge carrier transport and the optoelectronic properties of solar cells.

CPP 5.13 Tue 17:30 P

Self-assembled Hybrid Plasmonic Nanostructures for Perovskite Solar Cells — •TIANFU GUAN, RENJUN GUO, LENNART K. REB, SUZHE LIANG, CHRISTIAN L. WEINDL, WEI CAO, and PETER MÜLLER-BUSCHBAUM — Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany

Plasmonic metal-dielectric composites have gained great interest in various fields, owing to surface plasmon resonance (SPR) induced by incident radiation. The utilization of plasmonic metal nanoparticles (NPs) is frequently proposed as a means to further enhance the light absorption in the broad wavelength range as well as to facilitate charge collection and transport in the Perovskite solar cells (PSCs). To regulate the plasmonic spectral of Au NPs for maximizing the enhancement in light-absorption of the photoactive layer, we assembly the metal NPs onto the electron collecting layer to broaden the absorption band of the photoactive layer of optoelectronic devices as well as enhance the device performance. To meet the optimal results, we put effort into the plasmonic structure regulation, since the size, density, and morphology of the Au NPs will influence the crystallinity of the perovskite film and charge transportation of the device. GISAXS is used to study the quality of the plasmonic structure interface in terms of contact area with the perovskite film. GIWAXS is used to probe the crystalline structure of the perovskite active layers.

CPP 5.14 Tue 17:30 P

Effect of chemical modification on crystal structure and thermal properties of Polydiketopyrrolopyrrole Copolymers — •ROBERT KAHL¹, GERT KRAUSS², ANDREAS ERHARDT², OLEKSANDR DOLYNCHUK¹, MUKUNDAN THELAKKAT², and THOMAS THURN-ALBRECHT¹ — ¹Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany — ²Applied Functional Polymers, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany

Polydiketopyrrolopyrrole (PDPP) copolymers are second-generation semiconducting polymers that gained interest due to their superior performance in transistors and solar cells. Their chemical structure consisting of a DPP core with flanking units and/or co-monomers offers many opportunities to tune the optoelectronic properties by introducing chemical modifications. Here we investigated the thermal properties and crystal structure in bulk (DSC, TGA, WAXS) and in thin films (GIWAXS, AFM) of three PDPPs: PDPP[T]₂{2-HD}₂-T{DEG} (PDPP1) with thiophene flanking units and an additional OEG side chain, PDPP[Py]₂{2-HD}₂-T (PDPP2) with pyridine flanking units and PDPP[T]₂{2-HD}₂-T (PDPP3) with thiophene flanking units. PDPP3 shows only sanidic liquid crystalline order. PDPP1 shows crystalline order and a significantly lower melting temperature than PDPP2 and PDPP3. PDPP2 shows the most WAXS peaks, but has poor thermal stability. Our results demonstrate that thermal properties and ordering ability can be significantly influenced by introducing seemingly minor changes to the chemical structure of PDPPs.

CPP 5.15 Tue 17:30 P

Following the morphology formation of printed non-fullerene active layers for solar cells — •XINYU JIANG¹, SUO TU¹, MANUEL A. SCHEEL¹, SHANSHAN YIN¹, MATTHIAS SCHWARTZKOPF², STEPHAN V. ROTH^{2,3}, and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, Garching, Germany — ²DESY, Notkestr. 85, 22607 Hamburg, Germany — ³KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — ⁴Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Bulk heterojunction (BHJ) organic solar cells have gained significant improvements in the past few years, however, traditional laboratory deposition methods like spin coating are limited to small-scale production. Encouragingly, the emergence of printing techniques and the

development of in-situ observation technology open new windows for larger-area device manufacturing and inspection of the formation process of the printed active layer, respectively. We fabricate an active layer, which contains a donor polymer (PDTBT2T-FTBDT) and a non-fullerene acceptor (BTP-4F) with slot-die coating. The structure formation of the polymer domains is followed in-situ during the printing process with GIWAXS and UV-Vis spectroscopy measurements, respectively. Thus, structure evolution is coupled with optical properties during the printing process, thereby providing an understanding of the film formation kinetics of non-fullerene organic BHJ thin films.

CPP 5.16 Tue 17:30 P

Influence of non-halogenated solvents on the morphology and stability of PTQ10:BTP-4F organic solar cells — •LUKAS SPANIER¹, RENJUN GUO¹, JULIAN HEGER¹, YUQIN ZOU¹, MATTHIAS NUBER², MATTHIAS SCHWARTZKOPF³, DAVID TOTH⁴, RACHID HOUSSAINI⁴, HRISTO IGLEV², REINHARD KIENBERGER², ACHIM HARTSCHUH⁴, STEPHAN ROTH³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Lehrstuhl für Funktionelle Materialien, Garching, Germany — ²TU München, Lehrstuhl für Laser- und Röntgenphysik, Garching, Germany — ³Deutsches Elektronen-Synchrotron (DESY), FS-PE, Hamburg, Germany — ⁴Ludwig-Maximilians-Universität München, Department Chemie und CeNS, Munich, Germany

Organic solar cells (OSCs) have recently gained increasing attention due to their rapidly increasing efficiencies as well as the relatively easy scalability in their production. However, their manufacture relies heavily on the use of halogenated solvents, as organic solar cells made with environmentally friendly solvents often suffer from reduced performance. This can be partially reversed by raising the temperature of the solvents during formation of the bulk-heterojunction (BHJ).

We investigate and compare the changes in morphology and performance stability of PTQ10:BTP-4F OSCs processed from various solvents, utilising operando grazing-incidence X-ray scattering during illumination and solar cell operation. We further show the impact of solvent composition on the charge carrier dynamics in the respective BHJs using time-resolved transient absorption spectroscopy.

CPP 5.17 Tue 17:30 P

Polarization Resolved Optical Spectroscopy of PEN:PFP Charge-Transfer Excitons — •DARIUS GÜNDER¹, ANA M. VALENCIA^{2,3}, MICHELE GUERRINI^{2,3}, TOBIAS BREUER¹, CATERINA COCCHI^{2,3}, and GREGOR WITTE¹ — ¹Molekulare Festkörperphysik, Philipps-Universität Marburg — ²Institut für Physik, Carl von Ossietzky Universität Oldenburg — ³Physics Dept., Humboldt-Universität zu Berlin & IRIS Adlershof

Charge-transfer excitons (CTX) occurring at molecular donor/acceptor interfaces are considered important intermediates for charge separation in photovoltaic devices. Co-crystalline pentacene:perfluoro-pentacene (PEN:PFP) films can be prepared with different molecular orientation on SiO₂ and graphene substrates [1] and thus are well-suited model systems for detailed structure-property investigations of such CTX states. In this study, such crystalline PEN:PFP films with different molecular orientations are used to perform polarization and angular resolved UV/Vis absorption spectroscopy, in order to determine the direction of the transition dipole moment (TDM) of the CTX state, which is found to be perpendicular to the aromatic ring planes i.e. along the stacking direction. Interestingly, this orientation is different than for the singlet excitons of unitary acene films, which can be well-described by the Kasha-model using the TDMs of the single molecule HOMO-LUMO excitations that are oriented along the M-axis and thus constitutes an important benchmark system for a refined theoretical analysis of such molecular donor/acceptor systems. [1] D'Avino et al. Chem. Mater. 32, 3, 1261-1271 (2020)

CPP 5.18 Tue 17:30 P

Charge-transfer excitons in pentacene:perfluoropentacene co-crystal — •ANA M. VALENCIA GARCIA^{1,2}, DARIUS GÜNDER³, MICHELE GUERRINI^{1,2}, TOBIAS BREUER³, GREGOR WITTE³, and CATERINA COCCHI^{1,2} — ¹Institut für Physik, Carl von Ossietzky Universität Oldenburg — ²Physics Dept., Humboldt-Universität zu Berlin & IRIS Adlershof — ³Philipps-Universität Marburg, Molekulare Festkörperphysik, Marburg

Disclosing the nature of optical excitations in organic co-crystals is a challenge due to the complex interplay between the structural arrangement of the molecules and long-range electronic interactions in

these systems. For these reasons, the application of isolated cluster models is highly questionable. By means of density functional theory and many-body perturbation theory, we investigate the electronic and optical properties of the triclinic pentacene:perfluoropentacene co-crystal. The band-structure analysis indicates that the highest-occupied and the lowest-unoccupied states are mainly localized on different molecules, suggesting the presence of a charge-transfer exciton at the lowest energy, which is indeed revealed in the dielectric tensor computed from the solution of the Bethe-Salpeter equation. We demonstrate that this feature cannot be reproduced by a molecular cluster model where the first excitation is unambiguously polarized along the short molecular axis. Comparison with corresponding measurements clarifies the importance of adequate periodic treatment of molecular co-crystals to correctly reproduce the character of their excitations [1]. [1] Günder, Valencia, et al., in preparation.

CPP 5.19 Tue 17:30 P

Towards an accurate calculation of excitation energies of Bacteriochlorophyll complexes with Green's function-based many-body perturbation theory — ●ZOHREH HASHEMI¹ and LINN

LEPPERT^{1,2} — ¹Institute of Physics, University of Bayreuth, Germany — ²MESA+ Institute for Nanotechnology, University of Twente, Netherlands

Bacteriochlorophylls (BCL) are a family of chromophores with key functions in the primary energy-converting processes of bacterial photosynthesis. *In vivo*, BCLs are embedded in densely packed pigment-protein complexes; an accurate prediction of their electronic structure and excited states is key to understanding their interactions with each other and with their protein environment. However, the sheer size of these complexes, is presently an insurmountable challenge for highly accurate quantum chemical calculations.

Here we present calculations of the optoelectronic properties of BCL monomers and dimers based on first principles Green's function-based many-body perturbation theory within the *GW* and Bethe-Salpeter equation (BSE) approach. We find that optical excitations calculated with *GW*+BSE are in excellent agreement with experimental data and state-of-the-art wavefunction-based approaches - but achieved at considerably lower computational cost than the latter. Our study provides accurate reference results and highlights the potential of the *GW*+BSE approach for the simulation of larger pigment complexes.