

CPP 39: Organic Photovoltaics and Electronics II (joint session CPP/DS/HL, organized by HL)

Time: Wednesday 14:45–17:45

Location: POT 81

CPP 39.1 Wed 14:45 POT 81
singlet fission process of organic molecules attached to neon clusters — ●SHARAREH IZADNIA, AARON LAFORGE, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Charge and excitation transfer along with the corresponding decay and loss mechanism are fundamental aspects in light harvesting, organic photovoltaics, and optoelectronic devices.

In particular, singlet fission is a unique decay mechanism where a molecule excited to its singlet state can partially transfer its energy to a neighboring ground state molecule, and thereby create two molecules excited to a triplet state. As such, singlet fission can increase the efficiency of organic electronics and photovoltaic by creating multiple charge carriers from one single photon. Here, we report a systematic study of acene complexes attached to the surface of neon clusters. Depending on the system parameters, singlet fission and other lifetime reduction mechanisms are observed.

CPP 39.2 Wed 15:00 POT 81
Novel Organic NIR Detector Class Based on Charge-Transfer Absorption — ●BERNHARD SIEGMUND, ANDREAS MISCHOK, JOHANNES BENDUHN, OLAF ZEIKA, SASCHA ULLBRICH, FREDERIK NEHM, DONATO SPOLTRE, HARTMUT FRÖB, CHRISTIAN KÖRNER, KARL LEO, and KOEN VANDEWAL — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Dresden, Germany

Blending two organic species on a molecular level can introduce interfacial states which allow to absorb far below their optical gap. Although such intermolecular charge-transfer (CT) states form an important recombination path in organic solar cells, their near-infrared (NIR) absorption properties have been unused for photo-sensitive devices up to now. In this presentation, we disclose a new resonant optical cavity device architecture enabling NIR photodetection by means of efficient CT absorption. We demonstrate tunable detection wavelengths between 810nm and 1550nm with a single material blend, far below the optical gap of both donor and acceptor. The combination of spectral narrowband detection and broad tunability make this novel, flexible and potentially visibly transparent device principle highly suitable for integrated low cost spectroscopic NIR photodetection.

CPP 39.3 Wed 15:15 POT 81
Revealing the loss mechanisms in ZnO/organic hybrid solar cells — ●MORITZ EYER¹, SEBASTIAN KICKHÖFEL², JOHANNES FRISCH², SERGEY SADOFEV¹, JOACHIM PULS¹, NORBERT KOCH¹, EMIL LIST-KRATOCHVIL², and SYLKE BLUMSTENGEL² — ¹Institut für Physik, Humboldt-Universität zu Berlin — ²Inst. f. Physik, Inst. f. Chemie und IRIS Adlershof, Humboldt-Universität zu Berlin

In order to study the losses of ZnO/organic hybrid photovoltaic devices a model system of ZnMgO and poly(3-hexylthiophene) (P3HT) is introduced. It allows tuning the interface band gap energy between the ZnMgO conduction band minimum and the P3HT HOMO systematically by varying the Mg content in the inorganic component. This enables a profound study of charge separation and recombination processes at the interface of inorganic/organic hybrid heterojunctions.

Prior to full charge separation electron and hole on opposite sides of the interface form hybrid charge transfer excitons (HCTX) bound by Coulomb interaction [1]. Electroluminescence measurements in the near IR spectral range confirm the existence of HCTX and yield valuable information of their physical properties. Temperature dependent photovoltaic measurements provide the necessary information to understand the charge separation process and its influence on the parameters defining the performance of a photovoltaic device. A detailed study of the interface energetics allows quantifying the recombination losses of inorganic/organic hybrid heterojunctions in order to fully exploit their potential in solar energy.

[1] M. Eyer et. al. Appl. Phys. Lett. 107, 221602 (2015).

CPP 39.4 Wed 15:30 POT 81
Silver nanowires and polymer based transparent electrodes for Organic solar cells — ●YOONSEOK PARK, LUDWIG BORMANN, KOEN VANDEWAL, and KARL LEO — Dresden Integrated Center for

Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden, Germany

Organic photovoltaics (OPV) are prospective candidates for future renewable energy production because of their potential scalability, low cost, and flexibility. For establishing flexible organic devices, a highly transparent, conductive and flexible electrode is required, replacing ITO which is brittle and requires high temperature processes. Many alternative materials such as conductive polymers, graphene, and metal nanowires have been studied. Among these, metal nanowires, especially silver nanowire (AgNW) networks, show outstanding flexibility, conductivity, and transparency. However, AgNW network electrodes have a few basic problems: (i) a poor electrical contact between wires, resulting in a low conductivity, (ii) overlapping wires cause roughness, often resulting in electrical shorting of devices and (iii) open spaces between wires can be in the range of square micrometers. In this study, highly conductive PEDOT:PSS has been deposited on AgNW electrodes to form conductive bridges between the open spaces and to smoothen the sharp points of the network. The maximum process temperature is 120 °C. OPV cells using these AgNW / PEDOT:PSS transparent electrodes exhibit power conversion efficiencies up to 7.15%. Moreover, OPV devices on PET substrates with an alumina encapsulation and barrier adhesive show excellent mechanical flexibility.

CPP 39.5 Wed 15:45 POT 81
Three-dimensional graphene-based electrodes for asymmetric supercapacitors — ●MAXIMILIAN VON SECKENDORFF¹, SIMON DRIESCHNER¹, JÖRG WOHLKETZETTER¹, JOSE A. GARRIDO², and MARTIN STUTZMANN¹ — ¹Walter Schottky Institut und Physik-Department, Technische Universität München, Garching, Germany — ²The Barcelona Institute of Science and Technology, Bellaterra, Spain

Three-dimensional (3D) graphene-based structures combine the outstanding physical and chemical properties of graphene such as high conductivity, mechanical stability and chemical inertness with a high surface-to-volume ratio, making them highly promising for energy storage applications in supercapacitors. Here we demonstrate the fabrication of 3D graphene-based electrodes by chemical vapor deposition using sintered copper particles and electrodeposited nickel/copper alloys as catalytic metal substrates. After selective wet chemical etching of the metal scaffold, a freestanding graphene foam of high structural quality as confirmed by Raman spectroscopy is obtained. In an asymmetric supercapacitor, this graphene foam is used as the cathode and is combined with a graphene foam coated with pseudocapacitive elements such as manganese dioxide as the anode. This combination results in an extended electrochemical potential window above 1.5 V and, therefore, a higher energy density (> 5 Wh/kg) compared to symmetric supercapacitors. The electrochemical performance of this asymmetric capacitor is investigated by cyclic voltammetry, electrochemical impedance spectroscopy, and charge-discharge-measurements and confirms its great potential for energy storage applications.

Coffee Break

CPP 39.6 Wed 16:30 POT 81
Semitransparent Electrodes for Evaporated Small Molecule Organic Solar Cells — ●DHRITI SUNDAR GHOSH and KARL LEO — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), TU Dresden

Transparent Electrodes are key in novel flexible devices. We report a highly efficient microcavity assisted small molecule organic solar cell (SM-OSC), containing an indium-free semitransparent TiO₂(30nm)/Ag 9nm based transparent electrode with average visible transmittance of 66.7% and sheet resistance of 6.3 Ohm/sq. The electrode also consisted of a wetting layer of polyethyleneimine which promotes the growth of ultrasmooth, and highly conductive Ag films even at very low thicknesses. The role of high index TiO₂ undercoat layer is investigated in detail by optical simulations and is shown to enhance the microcavity effect, leading to increased light coupling into the photoactive layer. With comparable photocurrent, and high fill-factor values owing to much better electrical properties, the semitransparent electrode based SM-OSC outperforms the state-of-art indium tin oxide (ITO) based reference device with photon conversion effi-

ciency of 8.1% compared to 7.7% despite having lower transmittance ($\sim 21\%$) relative to ITO. This work demonstrates that a properly designed semitransparent TE is a promising alternative to ITO and can lead to more efficient photovoltaic devices.

CPP 39.7 Wed 16:45 POT 81

Intereference-induced thermoelectric effects in topological states of matter — ●FLAVIO RONETTI^{1,2}, LUCA VANNUCCI^{1,2}, GIACOMO DOLCETTO³, MATTEO CARREGA⁴, and MAURA SASSETTI^{1,2} — ¹Dipartimento di Fisica, Università di Genova, Via Dodecaneso 33, 16146, Genova, Italy. — ²CNR-SPIN, Via Dodecaneso 33, 16146, Genova, Italy. — ³Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg. — ⁴NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56127 Pisa, Italy.

In topological states of matter, such as edge states of quantum Hall systems and two-dimensional topological insulators, protection from backscattering guarantees phase-coherent ballistic transport, allowing for the observation of quantum interference effects. Intriguing thermoelectric properties can be achieved by exploiting the phase-coherent edge states of two quantum Hall systems coupled by tunnelling region. Considering a multiple quantum point contacts geometry, interference paths effectively break the electron-hole symmetry. Therefore, when the systems are driven out of equilibrium by a thermal gradient, a thermoelectric charge current can be induced. Correspondingly, an interference pattern in the heat current is predicted. In the case of two-dimensional topological insulators, the presence of spin degree of freedom give rise to a rich tunnelling dynamics. In a double quantum point contact geometry, the effective transmission related to spin-flipping processes acquires a functional dependence on energy in the interacting regime, thus generating a thermoelectric spin current in response to a thermal gradient.

CPP 39.8 Wed 17:00 POT 81

Organic thermoelectrics based on low-dimensional molecular metals — ●ALEXANDER STEEGER¹, FLORIAN HUEWE¹, and JENS PFLAUM^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Efficient recovery of waste heat by thermoelectric generators (TEGs) requires low-cost materials exhibiting high electrical conductivities σ and Seebeck coefficients S , but low thermal conductivities κ . The suitability of a given material for thermoelectric applications is quantified by the dimensionless figure of merit $zT = \sigma S^2 T / \kappa$. In this contribution, we propose crystalline low-dimensional molecular metals as an alternative class of organic thermoelectric materials combining the advantages of low weight, chemical variety, sustainability, high charge carrier mobility and reduced electronic dimensionality with the availability of p- and n-type conductors. For the first time, we determined all physical quantities contributing to zT on exclusively one single crystal sample of p-type TTT_2I_3 and n-type $(\text{DMe-DCNQI})_2\text{Cu}$, revealing high power factors and promising figures of merit surpassing $zT \geq 0.15$ below 40 K. The thermoelectric performance of low-dimensional metals is affirmed by the power output per active area of a prototypical all-organic TEG reaching values of $\sim \text{mW}/\text{cm}^2$ and could be further increased by taking full control over the amount of charge-transfer and band filling. Financial support by the DFG (Project No. PF385/6-1)

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CPP 39.9 Wed 17:15 POT 81

Ag-segregation at dislocations and grain boundaries in annealed PbTe thermoelectric materials studied by atom probe tomography — ●YUAN YU¹, OANA COJOCARU-MIRÉDIN¹, YARON AMOUYAL², ARIEL SHESKIN², and MATTHIAS WUTTIG¹ — ¹Physikalisches Institut (IA), RWTH Aachen, 52074, Aachen, Germany — ²Technion-Israel Institute of Technology, 32000 Haifa, Israel

PbTe-based alloys play a significant role in thermoelectric (TE) applications. The figure-of-merit, ZT , of standard PbTe is near 1, whereas for PbTe alloys doped with Sr, Na, K, and Ag, the ZT factors are larger than 2. The large enhancement of ZT values mainly benefits from the elemental doping-induced band modification and nano-precipitation. However, the effects of these dopants on the TE properties is still not well understood mainly due to the difficulty to track the impurity redistribution in 3D with traditional characterization techniques. Here, we investigated the distribution of Ag in PbTe TE material using 3D atom probe tomography. We clearly find that the Ag is prone to form platelet-like nanostructures with diameters of ~ 15 nm and thickness of ~ 3 nm in the as-quenched state. After annealing at 380°C for 48 h, these platelet-like nanostructures dissolve in the matrix, leading to a Ag-supersaturated matrix. Thus, the Ag tends to segregate at the dislocations and grain boundaries. These Ag-decorated dislocations and grain boundaries as well as the remaining stable Ag-rich nanoprecipitates are believed to influence the electron and phonon transport processes. Our results can help to better tailor the structures and provide more information for the theoretical calculation.

CPP 39.10 Wed 17:30 POT 81

Potassium Prussian Blue Nanoparticles: A Low-cost Cathode Material for Potassium-ion Batteries — ●YANG XU, MIN ZHOU, LIYING LIANG, and YONG LEI — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany

Potassium-ion batteries (KIBs) in organic electrolytes hold great promise owing to the abundance of potassium, close redox potential to lithium, and similar electrochemistry with lithium system. Investigations of KIB cathodes have been scarcely reported so far. We for the first time report hydrated potassium Prussian blue $\text{K}_0.220\text{Fe}[\text{Fe}(\text{CN})_6]0.805$ nanoparticles as a potential cathode material. The cathode exhibits a high discharge voltage of $3.1\sim 3.4$ V, high reversible capacity of 73.2 mAh g⁻¹, and great cyclability with a very small capacity decay rate of $\sim 0.09\%$ per cycle. Electrochemical reaction mechanism analysis identifies the carbon-coordinated FeIII/FeII couple as redox-active site and proves structural stability of the cathode during charge/discharge. Furthermore, we present a KIB full-cell by coupling the nanoparticles with commercial carbon materials. The full-cell delivers a capacity of 68.5 mAh g⁻¹ at 100 mA g⁻¹ and retains 93.4% of the capacity after 50 cycles. Considering the low cost and material sustainability, this work may trigger future attention on rechargeable KIBs.

Reference

C. Zhang, Y. Xu, M. Zhou, L. Liang, H. Dong, M. Wu, Y. Yang, Y. Lei, *Adv. Funct. Mater.* 2016, DOI: 10.1002/adfm.201604307.