

## HL 61: Posters III (Organic-inorganic perovskite semiconductors; Organic photovoltaics and electronics; Photovoltaics; Energy science; New materials and concepts)

Presenters are kindly requested to be near their poster for at least one hour in the time between 17:00-19:00 or to leave a note about their availability for discussions.

Time: Wednesday 15:00–20:00

Location: Poster F

HL 61.1 Wed 15:00 Poster F

### Processing influence on structural and electronic properties of Lead Methylammonium Tri-Iodide films —

•CHRISTIAN MÜLLER<sup>1,2,3</sup>, BERND EPDING<sup>1</sup>, ILKNUR YOLDAS<sup>2</sup>, ROBERT LOVRINCIC<sup>2,3</sup>, HANS-HERMANN JOHANNES<sup>2</sup>, and WOLFGANG KOWALSKY<sup>2,3</sup> — <sup>1</sup>Kirchhoff Institut für Physik, Universität Heidelberg — <sup>2</sup>Institut für Hochfrequenztechnik, TU Braunschweig — <sup>3</sup>InnovationLab GmbH, Heidelberg

Over the last few years the power conversion efficiency of organometal-halide perovskite (such as  $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) based solar cells has skyrocketed at an unprecedented rate to values around 18%. This development is even more impressive if we take into account that such high efficiencies can be reached for very different cell, made from different precursor materials, and for both solution and vacuum processed absorber layers. All this approaches have in common that the exact role of the perovskite microstructure for the device performance is to date not well understood. We focus in this work on a comparison between solution vs. vacuum processed perovskite layers and solar cells based thereon. SPM and SEM measurements were performed for the different perovskite films. Thereby we were able to map electronic and structural properties with high spatial resolution. This enables us to directly correlate the obtained data to the device performance.

HL 61.2 Wed 15:00 Poster F

### Charge Carrier Lifetime in methylammonium lead halide perovskite thin films —

•FABIAN MEIER, CORNELIUS KRASSELT und CARSTEN DEIBEL — Institute of Physics, Chemnitz University of Technology, 09126 Chemnitz, Germany

Thin film solar cells have shifted into the spotlight of current research and development because of their promising low-cost production resulting from high-throughput fabrication at low processing temperatures(1). Recently, hybrid perovskite structures on the base of lead halides have attracted considerable attention due to a tremendous increase in their power conversion efficiencies from 4% to nearly 18% within only a few years (2). Uncovering the recombination processes is of major importance for understanding and potentially circumventing the intrinsic losses in perovskite thin films. We performed absorption and photoluminescence (PL) measurements of both mixed and pure methylammonium lead halides. The comparably sharp onsets of absorption and emission as well as the small Stokes shift between them are signs for the small energy losses of the charge carriers within corresponding solar cells. The charge carrier decay dynamics were investigated by performing time-resolved PL decay by time correlated single photon counting. We will discuss our results in view of the role of free carrier recombination and trap assisted recombination.

(1)\*G.E. Eperon et al., *Adv. Funct. Mater.* 2014, 24, 151-157  
(2)\*N.G. Park, *Mater. Today* (2014), <http://dx.doi.org/10.1016/j.mattod.2014.07.001>

HL 61.3 Wed 15:00 Poster F

### Preparation and Characterization of Methylammonium Lead Iodide Perovskite Absorber Layers —

•DAVID GRABOWSKI, ANDREA JANSEN, LEVENT GÜTAY, STEPHAN J. HEISE, INGO RIEDEL, JÜRGEN PARISI, and HOLGER BORCHERT — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26129 Oldenburg, Germany

Since few years, perovskite thin films have attracted broad attention for application in solar cells: Without extreme efforts spent in technological developments, they already show strong electronic performance. In solar cells, the perovskite layer acts as a light absorber, that carries both electrons and holes. In this work we determine the significance of certain parameters during preparation on the emerging  $\text{CH}_3\text{NH}_3\text{PbI}_3$  perovskite film. Through means of scanning electron microscopy (SEM) and x-ray diffraction (XRD) a one-step method and a two-step method have been compared and the latter proved to be more effective to achieve the desired morphology and crystal structure. Therefore we utilize a two-step method to first apply  $\text{PbI}_2$  and later on  $\text{CH}_3\text{NH}_3\text{I}$  to create the perovskite, while systematically varying crucial parameters. Through means of the aforementioned measuring

equipment we verify advantageous parameters for mixing the solutions and the spin-coating process.

HL 61.4 Wed 15:00 Poster F

### Evaluation of different layer sequences of perovskite solar cells —

•ANDREA JANSEN, DAVID GRABOWSKI, DOROTHEA SCHEUNEMANN, MARIA S. HAMMER, INGO RIEDEL, JÜRGEN PARISI, and HOLGER BORCHERT — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26129 Oldenburg, Germany

Since few years, perovskite solar cells have attracted a massive increase in research effort, which is due to their potentially very high efficiencies at low costs. In solar cells the perovskite layer functions as a light absorber and exhibits the ability to transport both electrons and holes. In this work, the deposition of the perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$  was implemented via a two-step coating method, in which a solution containing  $\text{PbI}_2$  and another one containing  $\text{CH}_3\text{NH}_3\text{I}$  are deposited consecutively. Concerning photovoltaic performance, this method has shown to be advantageous compared to the one-step coating method, in which a solution containing both  $\text{CH}_3\text{NH}_3\text{I}$  and  $\text{PbI}_2$  is deposited on the substrate. The perovskite layers were analyzed by scanning electron microscopy (SEM) and X-ray diffraction (XRD), in order to determine the film morphology and crystal structure, respectively. Different device concepts for implementing the solution-cast perovskite layers into solar cells will be presented and discussed.

HL 61.5 Wed 15:00 Poster F

### First-principles study of tin-based hybrid organic-inorganic perovskites —

•JINGRUI LI and PATRICK RINKE — COMP / Department of Applied Physics, Aalto University, Finland

Hybrid organic-inorganic perovskites have received rapidly growing interest in recent years as promising photoactive materials in emergent solar cell technologies [1]. While much experimental work is conducted on hybrid perovskite devices, a quantum mechanical understanding of the basic materials properties and fundamental processes is lagging behind. In this work we present a first-principles study of a series of methylammonium tin trihalide ( $\text{CH}_3\text{NH}_3\text{SnX}_3$ ) perovskites employing relativistic density functional theory. We establish an all-electron reference for the ground state properties by benchmarking the local-atomic orbital code `FHI-aims` [2] and the full potential linear augmented plane wave code `exciting` [3] for the PBE exchange-correlation functional. The points of focus of our present study lie in (i) relativistic effects (more specifically, the scalar relativistic effects and the spin-orbit coupling) in the considered systems, (ii) improvement of electronic structure results by including exact exchange in the density functional, and (iii) changes in atomic and electronic properties due to the addition of halogenions into the organo-tin triiodide perovskite.

[1] See, e.g., M. A. Green *et al.*, *Nature Photon.*, **8**, 506 (2014).

[2] V. Blum *et al.*, *Comput. Phys. Commun.*, **180**, 2175 (2009).

[3] A. Gulans *et al.*, *J. Phys.: Condens. Matter*, **26**, 363202 (2014).

HL 61.6 Wed 15:00 Poster F

### Improved interfaces in solution processed perovskite solar cells —

•FLORIAN MATHIES<sup>1,3</sup>, JULIAN HEUSSER<sup>3,4</sup>, AINA QUINTILLA<sup>1</sup>, GUILLAUME GOMARD<sup>1</sup>, NORMAN MECHAU<sup>1,3</sup>, and ULI LEMMER<sup>1,2</sup> — <sup>1</sup>Light Technology Institute, Karlsruhe Institute of Technology, Germany — <sup>2</sup>Institute of Microstructure Technology, Karlsruhe Institute of Technology, Germany — <sup>3</sup>InnovationLab, Heidelberg, Germany — <sup>4</sup>Kirchhoff-Institute for Physics, University Heidelberg, Germany

Perovskite semiconductor materials promise to have a massive impact in the field of photovoltaics. Perovskite solar cells with efficiencies up to 19% have been recently fabricated, demonstrating their capability to compete with state-of-the-art silicon solar cells.

A critical point for the electrical performance in perovskite solar cells is the perovskite/metal oxide blocking layer interface. Consequently, we investigated different metal oxides ( $\text{TiO}_2$ ,  $\text{ZnO}$ , AZO and ZTO) with certain interfacial geometries, ranging from planar to nano-

mesoporous, with the perovskite layer. To make such solar cells compatible with flexible substrates and several industrially-relevant printing processes for a wide range of commercial applications, a reduction of process temperature is necessary. Using the previously described interfaces, the process temperature was reduced from 500°C to 120°C to determine its influence on the morphology at the interfacial layers by AFM and SEM studies, and on the electrical performance of the devices by IV-characteristic and IPCE measurements.

HL 61.7 Wed 15:00 Poster F

**Electrical Characterization of Methyl Ammonium Lead Iodide** — ●RAFFAEL RUESS, MARTINA STUMPP, CHRISTOPH RICHTER, PATRICK HOFMANN, and DERCK SCHLETTWEIN — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Methyl ammonium lead iodide ( $CH_3NH_3PbI_3$ ) is a trihalide perovskite semiconductor with promising and well-fitting parameters for the use as an absorber in hybrid solar cells. Homogeneous layers can be prepared by spin coating solutions of methyl ammonium iodide ( $CH_3NH_3I$ ) and lead iodide ( $PbI_2$ ) onto a substrate and annealing afterwards. In this work, the perovskite films were deposited via a two-step sequential deposition method. Current-voltage measurements were performed to determine the electrical conductivity of the perovskite film. An interesting hysteresis in the I-V measurements was observed corresponding to similar observations in perovskite solar cells and three possible reasons were discussed. Understanding the electrical behavior of perovskites, such as  $CH_3NH_3PbI_3$ , is important for finding further improvements on the efficiency of hybrid solar cells based on these materials.

HL 61.8 Wed 15:00 Poster F

**Replacement of Lead in Organic-Inorganic Perovskite Absorber Layers** — ●MANUEL WEISS, CHRISTOPH RICHTER, and DERCK SCHLETTWEIN — Institute of Applied Physics, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, D-35392 Gießen

Perovskite solar cells are a very promising low-cost technology as efficiencies around 20 percent have been reported. One problem, however, is the presence of lead in the cells. Lead is known to be a toxic heavy metal which is, therefore, banned from a number of technical applications in various countries which represent, however, important global markets. The presence of lead can therefore be seen as one major obstacle that could prevent the commercial use of perovskite solar cells. Alternative metal ions that are less toxic and abundant in the earth crust are sought to replace lead at maintained functionality of the films. In this contribution, alternative metal ions were tested to form organic-inorganic perovskite layers. Films were characterized by Scanning Electron Microscopy, UV-visible absorption spectroscopy, X-ray diffraction and XPS to probe the elemental composition, structure, morphology and electronic coupling in the films. The different materials will be discussed in their applicability as new absorber layers in perovskite solar cells.

HL 61.9 Wed 15:00 Poster F

**Current-Voltage Measurements on Perovskite Thin Films** — ●JAN TINZ, MARTINA STUMPP, CHRISTOPH RICHTER, PATRICK HOFMANN, and DERCK SCHLETTWEIN — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

The use of methyl ammonium lead iodide ( $CH_3NH_3PbI_3$ ) as light absorbing material enables the production of efficient and low-cost solar cells due to its high charge carrier mobility. The direct band gap of the perovskite can be controlled by replacing the iodide with bromide to optimize the light absorption. Thin films of  $CH_3NH_3Pb(I_{1-x}Br_x)_3$  were prepared in a one-step process by spin coating from solutions with different concentrations of lead iodide ( $PbI_2$ ), methyl ammonium iodide ( $CH_3NH_3I$ ) and methyl ammonium bromide ( $CH_3NH_3Br$ ) on these substrates. Depending on the concentration of the solution, the thickness of the synthesized perovskite films varied. Current-voltage measurements were performed and the electrical conductivity of the synthesized perovskite thin films was determined. A basic understanding of the electrical characteristics of these thin layers is required for the development of more efficient hybrid solar cells based on  $CH_3NH_3Pb(I_{1-x}Br_x)_3$ .

HL 61.10 Wed 15:00 Poster F

**Morphology of Methyl Ammonium Lead Iodide Thin Films Dependent on the Preparation Conditions** — MARTINA

STUMPP, ●JONAS HORN, RAFFAEL RUESS, JAN TINZ, and DERCK SCHLETTWEIN — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Solar cells based on perovskites as absorbing material have attained large attention in the last two years due to the strong increase in the efficiencies of these cells. Perovskites have the great advantage of a high charge carrier mobility, low non-radiative carrier recombination and strong solar absorption. In this study, thin films of methyl ammonium lead iodide ( $CH_3NH_3PbI_3$ ) were prepared by one- or two-step solution-based processes on different substrates. Profilometry measurements were performed to attain an understanding of the roughness and the thickness of the perovskite films. The detailed morphology of the films was analyzed with the help of laser confocal and scanning electron microscopy. The dependence of the different preparation methods as well as the use of different substrates on the morphology of the ( $CH_3NH_3PbI_3$ ) thin films is discussed.

HL 61.11 Wed 15:00 Poster F

**Processing Optimization for Vacuum Deposited Perovskite Layers** — ENKHTUR ERDENEBILEG, LAUREN E. POLANDER, CHRISTIAN KÖRNER, and ●KARL LEO — Institut für Angewandte Physik, Technische Universität Dresden, 01069 Dresden, Germany

Organic-inorganic hybrid perovskites currently attract considerable attention as promising light harvesting materials for solar cells due to their panchromatic absorption, excellent charge-transport characteristics, and ease of fabrication from inexpensive, commercially available materials. As a result of many recent advances related to changes in the stack design and processing conditions, the power conversion efficiency values for this new class of solar cells is increasing rapidly. Extremely uniform perovskite films can be formed using dual source vapor deposition of  $PbX_2$  and  $CH_3NH_3X$  (where  $X = I, Br, Cl$ ) to yield high performance devices when used in combination with either solution-processed or vacuum-deposited transport layers. In this work, we optimize the vapor deposition of perovskite layers by investigating the effects of evaporation and annealing temperature on the properties of isolated perovskite films. The films are thoroughly examined using UV-vis absorption spectroscopy, grazing incidence X-ray diffraction, and scanning electron microscopy. The newly developed deposition conditions are then applied to fabricate optimized perovskite solar cells with vapor-deposited electron- and hole-transport layers.

HL 61.12 Wed 15:00 Poster F

**Temperature-Dependence of a Perovskite-based Solar Cell** — ●HARALD HOPPE — Langewiesener Str. 22, Institut für Physik, TU Ilmenau

The temperature dependence of a solar cell based on a hybrid perovskite material has been investigated. We find distinctive changes to occur within the photovoltaic parameters with temperature variation. The results are discussed in view of structural and electronic data.

HL 61.13 Wed 15:00 Poster F

**Electroabsorption spectroscopy investigation of organic and perovskite solar cells** — ●CHENG LI<sup>1,3</sup>, YANA VAYNZOF<sup>2,3</sup>, TANAJI GUJAR<sup>1</sup>, DAN CREDGINGTON<sup>3</sup>, ZHI-KUANG TAN<sup>3</sup>, GIRISH LAKHWANI<sup>3</sup>, JIANPU WANG<sup>3,4</sup>, MUKUNDAN THELAKKAT<sup>1</sup>, NEIL GREENHAM<sup>3</sup>, and SVEN HÜTTNER<sup>1,3</sup> — <sup>1</sup>Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany — <sup>2</sup>Centre for Advanced Materials, Im Neuenheimer Feld 227, Heidelberg University, Heidelberg, 69120, Germany — <sup>3</sup>Cavendish Laboratory, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — <sup>4</sup>Institute of Advanced Materials, Nanjing Tech University, Nanjing, China 210009

In solution-processed photovoltaic devices, both organic and organic-inorganic perovskite based, the nanometer scale interfaces between the active material and electrodes play a crucial role on the device performance. In this poster, by using electroabsorption (EA) spectroscopy, combined with ultraviolet photoelectron spectroscopy (UPS), we investigate photovoltaic devices based on P3HT:PCBM, PBDTTT-CT:PC71BM and  $CH_3NH_3PbI_{3-x}Cl_x$  systems. As a non-invasive method, EA provides unique information of the built-in potential ( $V_{BI}$ ) in working devices. By characterizing the modulation of  $V_{BI}$ , we elucidate that the performance improvement of these solar cells utilizing interfacial engineering is mainly due to the shift of work function of electrodes, leading to an increase of the built-in potential in devices.

HL 61.14 Wed 15:00 Poster F

**Charge-transfer states vs. triplet excited states in organic**

**photovoltaics** — ●JOHANNES BENDUHN, DONATO SPOLTRE, CHRISTIAN KÖRNER, and KOEN VANDEWAL — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany  
Charge generation and recombination in organic solar cells occurs via the formation of charge-transfer (CT) states at the donor-acceptor interface. When the energy of the CT state is high, its formation can compete with the formation of triplet states on the donor or acceptor molecule, which can constitute an additional loss mechanism, reducing photo-voltaic performance.

With this work we aim to elucidate under which energetic and kinetic circumstances triplet state formation can be suppressed. Therefore we investigate material systems comprising of C<sub>60</sub> as acceptor and a series of phthalocyanine dyes with slight variations in their molecular structure (ZnPc, F<sub>4</sub> – ZnPc, CuPc, F<sub>4</sub> – CuPc) as donor. The addition of fluorine allows tuning of the energy of the CT state, resulting in an increased open circuit voltage. Varying the central atom from Zn to Cu enhances inter-system crossing to a triplet excited state on the phthalocyanine molecule. The energy levels of all relevant electronic excited states are determined by sensitive measurements of the external quantum efficiency spectrum. The formation of triplets is quantified by steady state photo-induced absorption at various temperatures.

We find that in the system with a reduced inter-system crossing, charge generation for materials with a high energy CT state is still efficient, even though the triplet state is the lowest energy state.

HL 61.15 Wed 15:00 Poster F

**Charge Transfer Absorption and Emission at ZnO/Organic Interfaces** — ●FORTUNATO PIERSIMONI<sup>1</sup>, RAPHAEL SCHLESINGER<sup>2</sup>, JOHANNES BENDUHN<sup>3</sup>, DONATO SPOLTRE<sup>3</sup>, SINA REITER<sup>1</sup>, ILJA LANGE<sup>1</sup>, NORBERT KOCH<sup>2</sup>, KOEN VANDEWAL<sup>3</sup>, and DIETER NEHER<sup>1</sup> — <sup>1</sup>Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Strasse 24-25, 14476 Potsdam, Germany — <sup>2</sup>Institut für Physik & IRIS, Adlershof Humboldt-Universität zu Berlin, Brook-Taylor-Strasse 6, 12489 Berlin, Germany — <sup>3</sup>Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

Here we investigate Hybrid Charge Transfer States (HCTS) at the planar interface based upon  $\alpha$ -NPD and ZnO by means of spectrally resolved electroluminescence (EL) and external quantum efficiency (EQE) measurements. The appearance of a sub-gap signal in the EL and in the EQE spectra proves respectively the radiative decay and the absorption from direct excitation of HCTSs. By means of various phononic acid based self-assembled monolayers we tune the ZnO work function and the energy gap (E<sub>gap</sub>) between the ZnO conduction band and  $\alpha$ -NPD LUMO level. We observe a correlation between E<sub>gap</sub>, the peak position of the NIR EL spectra and the open circuit voltage of photovoltaic devices, comprising these organic-inorganic interfaces. This unambiguously attributes the origin of the NIR emission to radiative recombination between an electron on the ZnO and a hole on  $\alpha$ -NPD and confirms the relation between open circuit voltage and the energy of the charge-state, also for hybrid organic-inorganic interfaces.

HL 61.16 Wed 15:00 Poster F

**Influence of electrical stress on the degradation of polymer solar cells** — ●TOBIAS FABER, ROLAND RÖSCH, and HARALD HOPPE — Institute of Physics, Ilmenau University of Technology, Langewiesener Straße 22, 98693 Ilmenau, Germany

The stability of polymer solar cells is an ever-present topic in today's research on organic photovoltaics. While protocols for stability testing have been established within the course of the International Summits on Organic Solar Cell Stability (ISOS), there is no consensus on the voltage range within which solar cells should be characterized during degradation experiments. We show that this open parameter can result in different effects on the degradation path and the amount of degradation. In-situ measurements of IV-characteristics of continuously illuminated *PCDTBT*:*PC70BM* solar cells were conducted every 30 minutes for about 1600 hours. Three different potential regimes were realized by applying three different voltage ranges: "forward voltage" (-0.1 V ... 5 V), "basic voltage" (-0.1 V ... 1 V) and "reverse voltage" (-5 V ... 1 V). A strong influence of the applied voltages and currents running through the device on the initial exponential decrease of the power conversion efficiency, the so-called "burn-in", was revealed. The origin of the differences is discussed and degradation pathways are suggested.

HL 61.17 Wed 15:00 Poster F

**Design of an energy-harvesting storage device based on or-**

**ganic solar cells and supercapacitor** — ●LUKAS HÖRLIN<sup>1</sup>, ANDREAS BAUMANN<sup>1</sup>, MATTHIAS WIENER<sup>1</sup>, GUDRUN REICHENAUER<sup>1</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Bayerisches Zentrum für Angewandte Energieforschung, Am Galgenberg 87, D-97074 Würzburg — <sup>2</sup>Experimentelle Physik 6, Julius-Maximilians-Universität Würzburg, Am Hubland, D-97074 Würzburg

A general problem of renewable energy system like photovoltaics and wind power is their volatility causing fluctuations in the power grid. Energy storage systems such as batteries or capacitors are promising candidates to overcome this fluctuations making use of renewable energy more reliably. We designed a small-scale energy-harvesting storage device, which demonstrates the storage and use of the redundant energy by photovoltaic devices, namely organic bulk heterojunction (BHJ) solar cells, in a supercapacitor for a certain period of time. State-of-the-art organic BHJ solar cells were prepared by spin-coating and characterized by means of current-voltage characteristics. The supercapacitor as the storage unit was analyzed by cyclic voltammetry. The energy harvesting system is realized by the ability to connect single organic solar cells in parallel and/or serial, which allowed us to vary the photocurrent and photovoltage of the unit and adapt it to the supercapacitor storage unit.

HL 61.18 Wed 15:00 Poster F

**Material properties of organo-halide perovskites at different temperatures** — ●GERHARD LACKNER<sup>1</sup>, IRINA ANUSCA<sup>1</sup>, VLADIMIR SHVARTSMANN<sup>1</sup>, MEHMET SANLIALP<sup>1</sup>, BRAHIM DHKIL<sup>2</sup>, and DORU C. LUPASCU<sup>1</sup> — <sup>1</sup>Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg\_Essen, Essen, Germany — <sup>2</sup>Ecole Centrale Paris, Structures, Properties and Modeling of Solids Laboratory, France

Recently, organo-halide perovskites have been attracted much interest by researchers due to their excellent performance as light absorbing material in solar cells. Certificated efficiencies of up to 20% have been reported [1]. Until now, the origins of their extremely well performance are not fully understood.

We investigated the material properties of methylammonium lead iodide (CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>) and methylammonium lead bromide (CH<sub>3</sub>NH<sub>3</sub>PbBr<sub>3</sub>) for different temperatures. The results of this study confirm these achieved by Mitzi [2].

[1] Press release 17.11.2014, Wirtschaftswoche green, Andreas Menn, last visited on 01.12.2014, available online: <http://green.wiwo.de/durchbruch-billig-solarzelle-erreicht-20-prozent-wirkungsgrad/>

[2] D. B. Mitzi, in Progress in Inorganic Chemistry, Vol. 48 (Ed.: K. D. Karlin), John Wiley & Sons, Inc. Hoboken, NJ, USA 1999, p. 1.

HL 61.19 Wed 15:00 Poster F

**Optoelectronic Interfaces for Restoration of Degenerated Retina** — ●OLIYA SADRILLAEVNA ABDULLAEVA<sup>1</sup>, MANUELA SCHIEK<sup>1</sup>, KARIN DEDEK<sup>2</sup>, MATTHIAS SCHULZ<sup>3</sup>, ARNE LÜTZEN<sup>3</sup>, and JÜRGEN PARISI<sup>1</sup> — <sup>1</sup>Energy and Semiconductor Research Laboratory, Department of Physics, Carl von Ossietzky University of Oldenburg, D-26111, Germany — <sup>2</sup>Department of Neurobiology, University of Oldenburg, 26111 Oldenburg, Germany — <sup>3</sup>Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

A novel approach towards the development of artificial photoreceptors for diseases like retinitis pigmentosa and age-related macular degeneration is the employment of organic semiconducting thin films. These conditions eventually cause blindness due to photoreceptor degeneration. Ghezzi et al. have recently reported the restoration of light in explanted retinas from animal models of photoreceptor degeneration by a single-component organic film of poly(3-hexylthiophene) via a photo-excitation process. They were able to trigger neuronal firing upon illumination. Our work focuses on employment of a Squaraine dye 2,4-Bis[4-(N,N-diisobutylamino)-2,6-dihydroxyphenyl]squaraine as potential organic material for neuronal stimulation. Squaraine dyes are characterized by their unique aromatic four membered ring system. This work is aimed at testing the biocompatibility of Squaraine dyes with different biological cell lines and if so exciting the cells by illumination.

HL 61.20 Wed 15:00 Poster F

**Band-like electron transport and high mobility in F<sub>2</sub>-TCNQ single-crystal field-effect transistors** — ●YULIA KRUPSKAYA<sup>1</sup>, MARCO GIBERTINI<sup>2</sup>, NICOLA MARZARI<sup>2</sup>, and ALBERTO MORPURGO<sup>1</sup> — <sup>1</sup>University of Geneva, Geneva, Switzerland — <sup>2</sup>EPFL, Lausanne,

Switzerland

It is believed that in organic single-crystal field-effect transistors (FET) of the highest quality, the electron transport occurs in the band-like regime, with the carrier mobility increasing upon lowering temperature. Neither the microscopic nature of this regime, nor why it occurs only in some materials but not in others is currently well understood. To address these issues, we performed a study of electron transport in single-crystal FET of different tetracyanoquinodimethane ( $F_x$ -TCNQ) molecules. We show that  $F_2$ -TCNQ devices exhibit the most pronounced band-like transport observed to date (a room-temperature electron mobility  $\mu = 6$ -7  $\text{cm}^2/\text{Vs}$ , increasing up to 25  $\text{cm}^2/\text{Vs}$  at 150 K), whereas in TCNQ and  $F_4$ -TCNQ FET  $\mu = 0.1$ -0.2  $\text{cm}^2/\text{Vs}$  at room temperature and decreases upon cooling. Moreover, we present a comparative analysis of the crystal structure, electronic structure and the electron-phonon interactions for the three studied materials aimed on understanding of the microscopic mechanisms responsible for so different transport properties.

Financial support: DFG KR 4364/1-1

HL 61.21 Wed 15:00 Poster F

**Polycyclic aromatic hydrocarbons in organic charge-transfer complexes** — ●SEBASTIAN WITT<sup>1</sup>, ANTONIA MORHERR<sup>1</sup>, MARTIN BAUMGARTEN<sup>2</sup>, ACHIM RIPPERT<sup>1</sup>, and CORNELIUS KRELLNER<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Goethe-Universität Frankfurt am Main — <sup>2</sup>Max-Planck-Institut für Polymerforschung, Mainz

Polycyclic aromatic hydrocarbons were discovered to present a new class of organic superconductors [1]. The organic molecules, as e.g. Picene, takes the role of an acceptor, when intercalated with alkali metals. We present the results of new organic charge-transfer complexes, where the polycyclic aromatic hydrocarbons could be either the donor or the acceptor. Applying the horizontal vapor growth in vacuum or in an inert gas we succeeded to co-crystallize seven new complexes. These single crystals were characterized by x-ray powder diffraction, single crystal Laue-type diffraction, in reflection and transmission, uv/vis-spectrometry and atomic force microscopy. In this contribution, we present the structural and physical properties of these new charge transfer complexes.

[1] R. Mitsuhashi *et al.*, Nature **464**, 74 (2010).

HL 61.22 Wed 15:00 Poster F

**Charge transfer and metallic conduction at the  $F_{16}\text{CoPc}$  - Rubrene interface** — ●FLORIAN RÜCKERL<sup>1</sup>, YULIA KRUPSKAYA<sup>2</sup>, ENI DODDIBA<sup>1</sup>, VASILIS NIKOLIS<sup>1</sup>, ALBERTO MORPURGO<sup>2</sup>, and MARTIN KNUPFER<sup>1</sup> — <sup>1</sup>IFW Dresden, Germany — <sup>2</sup>DPMC University of Geneva, Switzerland

We present the electronic properties of the  $F_{16}\text{CoPc}$ -Rubrene interface, studied by means of transport measurements and photoemission spectroscopy (PES). The interface (formed of  $F_{16}\text{CoPc}$  film evaporated on top of Rubrene single crystals) shows a slight metallic conductance at temperatures between 100 and 300 K with the resistivity of 300 k $\Omega$ , which is very low in comparison to previously studied organic interfaces [1] and lowest after the outstanding TTF-TCNQ interface [2]. Hall Effect measurements revealed the hole conductance in Rubrene with the hole density of  $1.6 \cdot 10^{13} \text{ cm}^{-2}$  and the mobility of 1.2  $\text{cm}^2/\text{Vs}$ . PES measurements at the interface with various layer thicknesses give clear evidence for a charge transfer. We observe an oxidation of the Rubrene molecules and a reduction of the Phthalocyanine Cobalt center by filling the  $3d_{z^2}$  orbital.

The very low resistivity and the fact that the magnetic Co ion is fully involved in the charge transfer process, makes this system especially interesting and promising in terms of organic electronics and molecular spintronics.

Financial support: KN 393/14, KR 4364/1-1

[1] I. Gutierrez Lezama *et al.* Nature Mat. 11, 588-794 (2012)

[2] H. Alves *et al.* Nature Mat. 7, 574-580 (2008)

HL 61.23 Wed 15:00 Poster F

**Charge Transfer at the Rubrene/ $F_{16}\text{CoPc}$  Interface Studied by X-ray Photoemission Spectroscopy and Near Edge X-ray Absorption Fine Structure** — ●JING GUO<sup>1</sup>, FLORIAN RÜCKERL<sup>2</sup>, FRANCIS HAIDU<sup>1</sup>, VOLODYMYR DZHAGAN<sup>1</sup>, GEORGETA SALVAN<sup>1</sup>, MARTIN KNUPFER<sup>2</sup>, and DIETRICH R. T. ZAHN<sup>1</sup> — <sup>1</sup>Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — <sup>2</sup>Leibniz Institute for Solid State and Materials Research Dresden, Electronic and Optical Properties Department, D-01069 Dresden, Germany

We studied the electronic properties of the  $F_{16}\text{CoPc}$ /rubrene interface using X-ray photoemission spectroscopy (XPS) and near edge X-ray absorption fine structure (NEXAFS). Due to the matching between the ionization potential of rubrene and the electron affinity of  $F_{16}\text{CoPc}$ , a charge transfer is expected to occur at the interface. Ferromagnetic LSMO layers were applied as substrates for the thin film growth due to potential spintronic application of such structures. The electron transfer from rubrene to the Co metal center is deduced from the lineshape of Co 2p band in the XPS spectra, resulting in a reduction of Co(II) to Co(I). NEXAFS data show a filling of the Co  $3d^2$  orbital of  $F_{16}\text{CoPc}$ , confirming the charge transfer. Besides, NEXAFS spectra show that  $F_{16}\text{CoPc}$  molecules have a tendency to stand on rubrene. The energy level alignment between rubrene and LSMO was also established using ultraviolet photoelectron spectroscopy and inverse photoemission spectroscopy

HL 61.24 Wed 15:00 Poster F

**Optical Spectroscopy on Organic-Inorganic Hybrid Structures - Charge Transfer in Type-II Level Systems** — ●INGO MEYENBURG<sup>1</sup>, BENJAMIN HEIDELMEIER<sup>1</sup>, MATTHIAS WEBER<sup>1</sup>, NILS ROSEMANN<sup>1</sup>, CHRISTIAN PRINZISKY<sup>2</sup>, JANE FALGENHAUER<sup>3</sup>, DERCK SCHLETTWEIN<sup>3</sup>, JÖRG SUNDERMEYER<sup>2</sup>, and WOLFRAM HEIMBRODT<sup>1</sup> — <sup>1</sup>Philipps Universität Marburg Department of Physics and Material Sciences Centre, Renthof 5, D-35032 Marburg — <sup>2</sup>Philipps Universität Marburg department of chemistry, Hans-Meerwein-Straße, D-35032 Marburg — <sup>3</sup>Justus-Liebig-University, Institute of Applied Physics, Heinrich-Buff-Ring 16, 35392, Gießen, Germany

Understanding interface processes is crucial for improvements of existing and new functional materials based on organic-inorganic hybrid semiconductor structures. Exciton recombination of spatially indirect excitons across type-II organic-inorganic interface can give access to the level alignment and interface properties of the hybrids. In addition to this method the depletion of excited organic states as a consequence of charge transfer into the inorganic semiconductor, which can be revealed by time resolved photoluminescence, can precise the determination of the level alignment. Further optical measurements including Raman spectroscopy help to understand the properties of hybrids including the interface. Starting with the idea of material combinations known from dye sensitized solar cells which imply a charge transfer from organic to inorganic structure some promising hybrid systems are investigated. Besides Antrachinone derivatives the indoline dye D149 on mesoporous ZnO is a recently studied hybrid structure.

HL 61.25 Wed 15:00 Poster F

**Investigation of Recombination Processes in Organic Solar Cells** — ●SASCHA ULLBRICH, DONATO SPOLTORE, JANINE FISCHER, CHRISTIAN KÖRNER, KOEN VANDEWAL, and KARL LEO — Institut für Angewandte Photophysik, Dresden, Deutschland

Recombination of charge carriers is one of the most important loss mechanisms in a solar cell. In competition to generation, it defines the open-circuit voltage by setting the equilibrium charge carrier density. Thus, it is necessary to study and understand recombination mechanisms in order to tap the full potential of organic photovoltaics. In this work, non-geminate recombination mechanisms and recombination dynamics of organic solar cells based on small molecules with different active layer thicknesses are studied. Charge extraction measurements and intensity dependent current-voltage characteristics are used to determine charge carrier densities, recombination rates and the dominant recombination mechanism under steady state conditions. We observe a change from bimolecular to trap-assisted recombination towards lower carrier densities and a decreasing recombination order with increasing active layer thicknesses.

HL 61.26 Wed 15:00 Poster F

**Effects of perfluorination on the electronic, optical, and transport properties of polyaromatic hydrocarbons: pentacene and pyrene in the molecular and solid phase** — ●ROBERTO CARDIA<sup>1</sup>, GIANCARLO CAPPELLINI<sup>1</sup>, and GIAN-MARCO RIGNANESE<sup>2</sup> — <sup>1</sup>Università di Cagliari and Istituto Officina dei Materiali-CNR, Italy — <sup>2</sup>Institute of Condensed Matter and Nanoscience, Université Catholique de Louvain, Belgium

We report a comparative study on pentacene and pyrene polyaromatic hydrocarbons (PAHs) and their perfluorinated counterparts. The study has been performed for both the isolated molecule and their molecular solid phases. The former are investigated, performing all-electron calculations, using Density Functional Theory (DFT) and Time Dependent DFT with localized gaussian basis set and hybrid

B3LYP exchange correlation functional, in order to quantify the effects of morphology and chemical modifications on their electronic, optical, and transport properties: in particular electron affinity, ionization energy, fundamental gap, optical absorption, exciton binding energy, and reorganization energies for holes and electrons. The molecular solids using DFT-LDA with plane-waves basis set and ionic pseudopotentials in order to determine and compare ground state properties. In contrast, different exchange-correlation functionals (LDA, PBE0) are considered to evaluate their electronic excitations.

HL 61.27 Wed 15:00 Poster F

**Comparison of the polarization-resolved linear absorption and time-resolved photoluminescence properties of crystalline perfluoropentacene on various substrates** — •DAVID LEIMBACH, ROBIN DÖRING, TOBIAS BREUER, GREGOR WITTE, and SANGAM CHATTERJEE — Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

Perfluoropentacene (PFP) is the perfluorinated counterpart and hence n-type organic semiconductor to the prototypical p-type pentacene. It can be grown as highly crystalline thin films on various optically transparent substrates such as NaF, KCl, and graphene. While PFP forms in the typical herringbone motif on both NaF and KCl, it shows a \*Brickwall\*-like polymorphism on graphene. Structural analyses show a  $\pi$ -stacking distance of only 3.07 Å [1], promising far higher values for electron and hole mobility and therefore greatly improved vertical transport, a desirable feature in potential organic electronic applications. Here, we investigate the influence of the packing motif and hence of the intermolecular coupling on the optoelectronic properties. Making use of polarization-resolved linear-absorption spectroscopy with sub- $\mu$ m spatial resolution we identify the corresponding exciton transition energies and correlate them with the orientation of crystalline domains and the substrate. Furthermore, we find altered carrier recombination dynamics using time-resolved micro-photoluminescence spectroscopy.

HL 61.28 Wed 15:00 Poster F

**Imaging the electric potential distribution of thin film solar cells** — •MICHAEL SCHERER<sup>1,2</sup>, ROBERT LOVRINCIC<sup>1,2</sup>, and WOLFGANG KOWALSKY<sup>1,2</sup> — <sup>1</sup>InnovationLab GmbH, Heidelberg — <sup>2</sup>TU Braunschweig, Institut für Hochfrequenztechnik, Braunschweig

Huge research efforts on second to fourth generation solar cells lead to a tremendous growth in the power conversion efficiency of thin film solar cells, competing silicon based photovoltaics.

Charge generation and transport in these devices occur in layered stacks containing thin films of different functional materials. Because of layer thicknesses on the nano- to microscale, a complex interplay of interface and bulk effects determines the performance of the devices. This interplay can hardly be predicted from simulations or interface experiments only, highlighting the role of cross-sectional studies with high lateral resolution. We perform a correlated scanning Kelvin probe microscopy (SKPM) and electron beam induced current (EBIC) study on solar cell cross sections to image the electronic properties of entire solar cell devices.

Our scanning probe station is placed within the vacuum of a combined scanning electron microscopy (SEM)/focused ion beam (FIB) cross beam system. We prepare cross sections of different types of solar cells and characterize them with SKPM and EBIC on the same spot. The samples are illuminated and contacted in a defined manner and studied in vivo within the vacuum of our cross beam station.

HL 61.29 Wed 15:00 Poster F

**Influence of ZnO doping in ALD deposited Al<sub>2</sub>O<sub>3</sub> on Q<sub>fix</sub> and charge carrier lifetime** — •JOHANNES ZIEGLER<sup>1</sup>, THOMAS SCHNEIDER<sup>1</sup>, ALEXANDER N. SPRAFKE<sup>1</sup>, and RALF B. WEHRSPÖHN<sup>1,2</sup> — <sup>1</sup>Institute of Physics Martin Luther University Halle-Wittenberg — <sup>2</sup>Fraunhofer Institute for Mechanics of Materials IWM Halle

Thin Al<sub>2</sub>O<sub>3</sub> films deposited by thermal ALD on Si surfaces are known to provide an excellent passivation quality. Beside the chemical passivation of recombination active dangling bonds on the silicon surface by saturation, the field effect passivation generated by a high density of fixed negative charges in the Al<sub>2</sub>O<sub>3</sub> is responsible for the reduction of parasitic charge carrier recombination in silicon solar cells [1]. In this work the influence of ZnO on the fixed negative charges in the Al<sub>2</sub>O<sub>3</sub> layers and on their passivation quality on p-type silicon is studied by CV and QSSPC measurements.

[1] B.Hoex, J.Schmidt, R.Bock, P.P. Altermatt, M. C. M. van de Sanden and W. M. M. Kessels, Appl. Phys. Lett, 89:042112 (2006)

HL 61.30 Wed 15:00 Poster F

**Investigation of order-disorder related band gap changes in Cu<sub>2</sub>ZnSn(S,Se)<sub>4</sub> solar cells using electroreflectance** — CHRISTOPH KRÄMMER<sup>1</sup>, CHRISTIAN HUBER<sup>1</sup>, CHRISTIAN ZIMMERMANN<sup>1</sup>, MARIO LANG<sup>1</sup>, •ALEXANDER OPOLKA<sup>1</sup>, THOMAS SCHNABEL<sup>2</sup>, TOBIAS ABZIEHER<sup>1,2</sup>, ERIK AHLSEDE<sup>2</sup>, HEINZ KALT<sup>1</sup>, and MICHAEL HETTERICH<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — <sup>2</sup>Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany

Cu<sub>2</sub>ZnSn(S,Se)<sub>4</sub> (CZTSSe) has attracted attention in thin-film photovoltaics due to its similarity to the well-established Cu(In,Ga)(S,Se)<sub>2</sub>. However, the use of the low-cost and earth-abundant constituents Zn and Sn promise to overcome the weak point of the Cu(In,Ga)(S,Se)<sub>2</sub> system, although up to now the gap in efficiency between these two systems could not be closed. Among other things a high amount of point defects is made responsible for this deficit. In this contribution we demonstrate reversible band gap shifts which are induced by post-annealing of finished CZTSSe solar cells and are attributed to changes in the disorder within the Cu-Zn lattice planes. These changes follow the stochastic Vineyard model which further predicts a critical temperature above which the kesterite structure is entirely Cu-Zn disordered.

HL 61.31 Wed 15:00 Poster F

**Photoluminescence investigation of the order-disorder effect in Cu<sub>2</sub>ZnSn(S,Se)<sub>4</sub> solar cells** — CHRISTIAN ZIMMERMANN<sup>1</sup>, •MARIO LANG<sup>1</sup>, CHRISTOPH KRÄMMER<sup>1</sup>, THOMAS SCHNABEL<sup>2</sup>, TOBIAS ABZIEHER<sup>1,2</sup>, ANGELIKA SCHULZ<sup>1</sup>, HEINZ KALT<sup>1</sup>, and MICHAEL HETTERICH<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — <sup>2</sup>Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany

Due to its composition of low-cost and earth-abundant elements, Cu<sub>2</sub>ZnSn(S,Se)<sub>4</sub> (CZTSSe) is a promising material system for thin-film photovoltaics. Yet, a lack of efficiency compared to the well-established thin-film technology Cu(In,Ga)(S,Se)<sub>2</sub> is present, and therefore further improvements have to be realized. Recently, an order-disorder transition accompanied by a band gap shift has been reported. In this contribution the influence of this transition on the photoluminescence spectra is investigated as a function of sample temperature and excitation power. The results are analysed with reference to the fluctuating potential model.

HL 61.32 Wed 15:00 Poster F

**Solution-based fabrication of kesterite Cu<sub>2</sub>ZnSnSe<sub>4</sub> absorber layers and solar cells** — •MARKUS NEUWIRTH<sup>1</sup>, HUIJUAN ZHOU<sup>1</sup>, CHAO GAO<sup>1</sup>, MARIO LANG<sup>1</sup>, CHRISTIAN ZIMMERMANN<sup>1</sup>, CHRISTOPH KRÄMMER<sup>1</sup>, CHRISTIAN HUBER<sup>1</sup>, ALEXANDER SCHIELE<sup>1</sup>, THOMAS SCHNABEL<sup>2</sup>, TOBIAS ABZIEHER<sup>2</sup>, ERIK AHLSEDE<sup>2</sup>, MICHAEL POWALLA<sup>2,3</sup>, HEINZ KALT<sup>1</sup>, and MICHAEL HETTERICH<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — <sup>2</sup>Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany — <sup>3</sup>Light Technology Institute, KIT

In the race for new energy sources, Cu<sub>2</sub>ZnSnSe<sub>4</sub> (CZTSe) thin-film solar cells play a promising role since the absorber only comprises environmentally friendly and earth-abundant elements. Our fabrication approach for CZTSe consists of a cheap and simple solution-based two-step process that spares toxic solvents such as hydrazine. Utilizing a doctor-blading process we are able to form reproducible homogeneous precursors that transform into CZTSe by subsequent thermal annealing in a Se atmosphere. An automated buffer layer deposition process also increases the reproducibility of the overall sample quality. X-ray diffraction, Raman spectroscopy and external quantum efficiency measurements provide a better understanding of the kesterite absorber properties and their influence on cell performance.

HL 61.33 Wed 15:00 Poster F

**Two-step fabrication process for Cu<sub>2</sub>ZnSnSe<sub>4</sub> layers and solar cells on GaAs and molybdenum-coated glass substrates** — •ALEXANDER SCHIELE<sup>1</sup>, CHAO GAO<sup>1</sup>, MARIO LANG<sup>1</sup>, CHRISTOPH KRÄMMER<sup>1</sup>, THOMAS SCHNABEL<sup>2</sup>, TOBIAS ABZIEHER<sup>2</sup>, ERIK AHLSEDE<sup>2</sup>, HEINZ KALT<sup>1</sup>, and MICHAEL HETTERICH<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, Karlsruhe Institute of Technology (KIT),

76131 Karlsruhe, Germany — <sup>2</sup>Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany

$\text{Cu}_2\text{ZnSnSe}_4$  (CZTSe) is a promising thin-film absorber material due to its earth-abundant, low-cost and non-toxic components. Despite these advantages, CZTSe solar cells have not yet achieved the required efficiency for practical application. Therefore, high-quality absorber layers are necessary in order to perform fundamental material studies and further improve device performance. One way of fabricating such high-quality CZTSe layers is to utilize a precursor layer stack consisting of (epitaxial) ZnSe, Cu, and Sn deposited in a molecular-beam epitaxy system. A subsequent annealing process leads to the formation of CZTSe with large grains which in case of a GaAs(001) substrate inherits the preferential orientation of the monocrystalline ZnSe layer. The influence of GaAs as a substrate compared to molybdenum-coated glass is investigated by X-ray diffraction, Raman spectroscopy, and conversion efficiency measurements of finished solar cells.

HL 61.34 Wed 15:00 Poster F

**Development and Characterization of an Ultrathin Hybrid p-n Interface for Solar Cell Applications** — ●MAHFUJUR RAHAMAN, RAUL D. RODRIGUEZ, JACEK GASIOROWSKI, and DIETRICH R. T. ZAHN — Halbleiterphysik, Technische Universität Chemnitz, Germany  
In this work ultra-thin hybrid p-n interfaces were developed and characterized for photovoltaic application using inorganic 2-dimensional p-type GaSe as well as F16CoPc and PCBM n-type organic semiconductors. Due to the layered structure of GaSe, it is possible to deposit nano flakes by means of mechanical exfoliation. The F16CoPc thin film was deposited by thermal evaporation and PCBM by spin coating on a metal substrate. The properties of p-n interfaces were determined using a wide spectrum of techniques. Optical properties were characterized using spectroscopic ellipsometry (SE) and photoluminescence, while the surface morphology and electrical studies were performed using atomic force microscopy (AFM) and Kelvin probe force microscopy (KPFM) methods. The photovoltaic effect was investigated by means of I-V measurements in the dark and under illumination using 514.7 nm laser excitation.

HL 61.35 Wed 15:00 Poster F

**Time-resolved Photoluminescence in thin film semiconductors - experiment and simulation** — MATTHIAS MAIBERG, CONRAD SPINDLER, TORSTEN HÖLSCHER, ENRICO JARZEMBOWSKI, STEFAN HARTNAUER, and ●ROLAND SCHEER — Martin-Luther-University Halle-Wittenberg, Photovoltaics Group, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Time-resolved photoluminescence (TRPL) often is used to measure the effective lifetime of minority carriers in a semiconductor. However, there are several reasons for the TRPL decay not equal the decay of the minority carrier density: Bimolecular recombination, charge carrier drift and diffusion, shallow defects in the band gap, and varying defect densities.

By computer simulation we can explain most of the experimental findings. A curved decay for excitation with high injection levels can be assigned to bimolecular recombination. Contrary, a curved decay for low injection levels can be related to minority carrier capture and reemission from shallow defects in the band gap as well as to defect densities that vary on the lateral scale.

In bias voltage dependent TRPL on pn junctions (solar cells), the decay time increases with increasing voltage. This can be explained by a reduction of charge carrier drift in the space charge region and may be used to determine the charge carrier mobility.

HL 61.36 Wed 15:00 Poster F

**Optical Imaging of Cu(In,Ga)Se<sub>2</sub> Solar Cells with Consideration of Material Homogeneity as a Quality Control Tool for Photovoltaic Devices** — ●STEFFEN KRETZSCHMAR, OLIVER NAGEL, DIETER GREINER, CHRISTIAN A. KAUFMANN, and THOMAS UNOLD — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, D-14109 Berlin

The luminescence yield of Cu(In,Ga)Se<sub>2</sub> solar cells or absorber layers can be used as a quality control indicator of the photovoltaic performance, in particular the open circuit voltage, of these devices. Here we present a study of electroluminescence and photoluminescence imaging on Cu(In,Ga)Se<sub>2</sub> solar cells using an InGaAs detection system with a good spectral match to the chalcopyrite luminescence emission. The results are compared to current-voltage and external quantum efficiency

analyses on the same devices. In accordance with theory we find a linear dependence of the open circuit voltage on the logarithm of the luminescence yield. However, when not taking lateral inhomogeneities into account, a large spread in the correlation of solar cell parameters to imaging results is observed. We find that using an analytical homogeneity correction model leads to a distinct improvement of the correlation between the luminescence data and the device parameters open-circuit voltage and conversion efficiency which allows the use of luminescence imaging as a predictive tool for inline monitoring and quality control.

HL 61.37 Wed 15:00 Poster F

**First-principles calculation of the band alignment of Cu-GaS<sub>2</sub> chalcopyrite for photovoltaic purpose** — JESUS EDUARDO CASTELLANOS<sup>1,2</sup>, ●PABLO PALACIOS<sup>1,3</sup>, JESUS J. ARRIAGA<sup>2</sup>, and PERLA WAHÓN<sup>1</sup> — <sup>1</sup>Instituto de Energía Solar, ETSI Telecomunicación, Universidad Politécnica de Madrid, 28040 Madrid, Spain. — <sup>2</sup>Instituto de Física, Benemérita Universidad Autónoma de Puebla, Av. San Claudio y 18 Sur. C.U. 72570. Puebla, México — <sup>3</sup>Dpt. Física Aplicada a las ingenierías Aeronáutica y Naval, ETSIAE, Universidad Politécnica de Madrid, 28040, Madrid, Spain.

The study of interfaces between two materials semiconductors, being one of them the CuGaS<sub>2</sub> chalcopyrite, and the processes that occurs in the interfaces are necessary for a better understanding of how these proposed materials operate in the entire structure of the solar cell. In our study we considered the effect of the lattice mismatch between each pair of contact materials. We search for surface orientations which can reduce as most as possible the lattice mismatch, but strained layer have appeared. This strain has an important effect on the electronic structure, mainly in the band-gap. Alignments are calculated using the electrostatic potential as reference. Using the periodic slab model we calculated the minimum-energy structure and band offset for the three specific interfaces. Some of these interfaces have shown band alignments which are suitable for potential applications in photovoltaics and optoelectronics.

HL 61.38 Wed 15:00 Poster F

**Microstructure Investigation of Lithiated Silicon** — ●WENLONG ZHAO, LUKAS DIEKMAYER, EIKE EPLER, BURKHARD ROOS, VLADIMIR RODDASIS, CYNTHIA A. VOLKERT, and CARSTEN NOWAK — Insitute for Materials Physics, Göttingen, Germany

Because of its theoretically high gravimetric capacity, silicon receives a lot of attention as potential anode material for lithium-ion batteries. Experimentally, the expected capacity is usually not observed which is attributed to the high volume change of silicon on lithiation and the accompanying amorphization of the silicon.

In this work, we present results on the microstructure investigation of lithiated silicon. Single crystalline silicon pillars of micrometer dimension were electrochemically lithiated in an organic electrolyte. After subsequent delithiation and focused ion beam based sample preparation, the samples were characterized with high resolution transmission electron microscopy and laser assisted atom probe tomography. The observed formation of atomic scale defects on {111} and {113} planes and the formation of amorphous channels in the volume of the material are discussed.

HL 61.39 Wed 15:00 Poster F

**Transport Measurements on Thermoelectric CoSb<sub>3</sub> and Partially-Filled Yb<sub>x</sub>Co<sub>4</sub>Sb<sub>12</sub> Skutterudites** — ●MARTIN LONSKY<sup>1</sup>, SVEN HEINZ<sup>1</sup>, MARCUS DANIEL<sup>2</sup>, MANFRED ALBRECHT<sup>2,3</sup>, and JENS MÜLLER<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Goethe-Universität, Frankfurt (M), Germany — <sup>2</sup>Institut für Physik, TU Chemnitz, Chemnitz, Germany — <sup>3</sup>Institut für Physik, Universität Augsburg, Augsburg, Germany

Semiconducting CoSb<sub>3</sub> is a member of the skutterudite family of compounds and a promising candidate for thermoelectric applications. Its thermoelectric properties can be improved by filling void space in its crystal structure with foreign atoms such as Yb or La. These loosely bound atoms serve as phonon-scattering centers and thereby reduce thermal conductivity drastically.

The aim of our study is a systematic investigation of the electronic transport properties for different filling factors on thin films of thermoelectric CoSb<sub>3</sub> and partially filled Yb<sub>x</sub>Co<sub>4</sub>Sb<sub>12</sub> skutterudites. Transport parameters as resistivity  $\rho(T)$ , effective charge carrier density  $n(T)$  and Hall mobility  $\mu(T)$  have been determined in a broad temperature range from 20 to 250 K. In contrast to CoSb<sub>3</sub>, which is close to compensation of hole- and electron-like carriers, Yb<sub>x</sub>Co<sub>4</sub>Sb<sub>12</sub> clearly

shows an n-type semiconductor behavior. Apart from resistance and Hall-effect measurements, we applied fluctuation (noise) spectroscopy in order to gain a deeper insight into the charge carrier dynamics of the investigated materials.

HL 61.40 Wed 15:00 Poster F

**In situ Raman investigation of silicene** — ●DMYTRO SOLONENKO<sup>1</sup>, PATRICK VOGT<sup>2</sup>, OVIDIU D. GORDAN<sup>1</sup>, and DIETRICH R. T. ZAHN<sup>1</sup> — <sup>1</sup>Halbleiterphysik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — <sup>2</sup>Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany

Silicene, the silicon counterpart of graphene, possesses unique electronic and structural properties. Its inherent buckling leads to an opening of the bandgap and presence of polarized spin-states under an external electric field[1]. Moreover, its implementation into Si-based technology is considered to be less challenging than in the case of graphene. Silicene does not exist in nature and can be obtained only by synthesis on a supporting substrate. Only recently silicene could be synthesized on Ag(111) and characterized in terms of its structural and electronic properties[2]. However, some questions regarding the structural aspects and the interaction with the Ag substrate remain. Raman spectroscopy was employed to answer some of the open questions. Here, we report in situ Raman measurements of mono- and multilayer silicene obtained for a broad range of excitation wavelengths. Silicene layers were grown under UHV-conditions on a Ag (111) substrate and the formation of different silicene phases was verified by LEED. The temperature and chemical stability of silicene was tested by in situ temperature-dependent measurements and ex situ oxidation.

1. N.D. Drummond et al., Physical Review B 85, (2012).
2. P. Vogt et al., Physical Review Letters 108, (2012).

HL 61.41 Wed 15:00 Poster F

**Coulomb oscillations in improved metal nanoparticle field-effect transistors** — ●SVENJA WILLING, MIRJAM VOLKMANN, SANDRA MÖLLER, HAUKE LEHMANN, and CHRISTIAN KLINKE — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Following the current down-scaling trend in electronic device

fabrication, transistors based on nanoparticles represent a great possibility for further miniaturization. The small self-capacitance of the individual metal nanoparticles results in a Coulomb energy gap [1] that is influenced not only by the particles' size and interparticle distance but also by electrical fields. The transport through arrays of metal nanoparticles separated by tunnel barriers can thus be tuned through the application of a gate voltage in the manner of a conventional semiconductor field-effect transistor.

We synthesize monodisperse CoPt nanoparticles by colloidal chemistry [2] and deposit them onto silicon substrates as highly-ordered monolayers via the scalable Langmuir-Blodgett method. Using standard lithography steps, we implement different gate geometries and define the shape of the nanoparticle array to improve the gate-voltage influence in the resulting metal nanoparticle based transistor. Electrical transport measurements show a broad Coulomb blockade regime and Coulomb oscillations in the output and transfer characteristics respectively. We find that the oscillations can be measured at temperatures of up to approximately 100 K.

- [1] Phys. Rev. B **44**, 1646 (1991) [2] Nano Lett. **10**, 964 (2010)

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**Study of CIS/ZnO heterojunction solar cells by electrical characterization** — ●JAIRO CESAR NOLASCO, DOROTHEA SCHEUNEMANN, HOLGER BORCHERT, and JÜRGEN PARISI — Energy and Semiconductor Research Laboratory, Department of Physics, Carl von Ossietzky University of Oldenburg, D-26111, Germany

Colloidal quantum dot (CQD) photovoltaics, using solely solution-processed semiconductor nanocrystals as light-harvesting material, have seen rapid advances in recent years. The use of highly toxic Pb and Cd compounds used in absorber films, such as PbSe and PbS might limit the possible application of CQD photovoltaics. It has been demonstrated, that one less toxic alternative is the use of CuInS<sub>2</sub> (CIS) as absorber material. Initial studies on CIS/ZnO heterojunction solar cells indicated that their performance is limited by an interface barrier. In this contribution, by using electrical characteristics (e.g., capacitance-voltage measurements) and device modeling, the existence of such heterojunction interface barrier is investigated.