HL 72: Poster Session: Si-based Photovoltaics / Inorganic Photovoltaics / Structure and Transport in Organic Photovoltaics / Organic Semiconductors

Time: Wednesday 16:00–19:00 Location: Poster D

HL 72.1 Wed 16:00 Poster D

Porous silicon antireflective layer fabricated by platinum nanoparticle assisted chemical etching — •Xiaopeng Li[1], Stefan Schweizer[2], and Ralf Wehrspohn[3] — [1]Max-Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Germany — [3]Fraunhofer Institute for Mechanics of Materials at Halle, Germany

Meal assisted chemical etching (MaCE), is a purely solution processed, high throughput technique. Si wafers loaded with metal nanoparitcles (NPs) such as Ag, Au or Pt, are immersed in solution containing HF and an oxidant. Etching preferentially occurs beneath the metal NPs, enabling the formation of nanopores and nanowires. Here, we presented for the first time, the formation of uniform porous silicon layer with pore size ranging from meso- to macro-size, by using platinum nanoparticle assisted chemical etching (PaCE). Various factors influencing the porous silicon morphology including PtNP density, silicon doping level, and H2O2 concentration were systematically studied. A new etching mechanism was evaluated. The formed macroporous Si showed the reflectance below 2.5% at the wavelength range of 300 nm to 1000 nm, and mesoporous Si exhibited broadband light absorption, even in the near infrared range. With perfect light trapping, macroporous silicon demonstrated more than 10 mA/cm2 photocurrent increase than that of controlled planar Si samples.

HL 72.2 Wed 16:00 Poster D

Absorption properties of femtosecond laser microstructured Black Silicon for solar cell application — •Anna Lena Baumann[1], Kay-Michael Guenther[2], Thomas Gimpel[2], Stefan Kontermann[1], Philipp Saring[3], Michael Seibt[3], and Wolfgang Schade[1,2] — [1]Fraunhofer Heinrich Hertz Institute, EnergieCampus, Am Stollen 19B, 38640 Goslar — [2]Clausthal University of Technology, EFZN, EnergieCampus, Am Stollen 19B, 38640 Goslar — [3]Georg-August-Universität Göttingen, IV. Physikalisches Institut, Semiconductor Physics, Friedrich-Hund-Platz 1, 37077 Göttingen

First deep-level transient spectroscopy (DLTS) measurements indicate the presence of sulfur energy levels in the band gap of femtosecond laser microstructured Black Silicon. Samples featuring different energy levels in DLTS measurements show different absorption properties as well. One way to influence the absorption values and the sulfur energy levels in Black Silicon is an additional post-laser process annealing step. This decreases the infrared absorption and shifts the sulfur energy levels to different values. Another way to affect the Black Silicon absorption works by changing the laser pulse shape. Preliminary double pulse experiments yield samples with different absorption in the near infrared when varying the double pulse distance. Modifying the pulse shape seems to be a promising method to influence absorption properties along with sulfur energy levels in Black Silicon.

HL 72.3 Wed 16:00 Poster D

Black Silicon solar cell emitter doping concentration measured with impedance spectroscopy — •Kay-Michael Günther[1], Alexander Bomm[2], Thomas Gimpel[1], Stefan Kontermann[2], and Wolfgang Schade[1,2] — [1]Clausthal University of Technology, EFZN, Am Stollen 19B, 38640 Goslar, Germany — [2]Fraunhofer Heinrich Hertz Institute, Am Stollen 19B, 38640 Goslar, Germany

Exposing silicon to femtosecond-laser pulses leads to a nanostructured surface which features an enhanced light absorption. Therefore, this material is called Black Silicon. When the laser processing is performed under a sulfur-containing atmosphere, sulfur is incorporated in the silicon lattice. Secondary ion-mass spectroscopy (SIMS) shows that the silicon contains up to 0.5 at% sulfur. A pn-junction is formed for p-type base material which can be used for solar cell applications. For a solar cell solely based on Black Silicon we achieved a record efficiency of 4.5%. Nevertheless, for a device optimization the uncompensated donor concentration has to be determined. We use capacitance-voltage (C-V) measurements for obtaining the doping profiles of our samples. Because of the structured surface and the pn-junction, conventional C-V methods cannot be applied due to the interfering space charges. Therefore, we use a new method which is based on impedance spectroscopy. We can show that only a small fraction of the sulfur is electrically active and acts as a donor.

HL 72.4 Wed 16:00 Poster D

Solution-processed silicon particle semiconductor films — •Sara Jäckle[1,2], Ralf Krause[1], and Hans-Ulrich Krebs[2] — [1]Günther-Scharowsky-Str.1, 91058 Erlangen — [2]Institut für Materialphysik, Universität Göttingen

Conventional PV-modules are mostly based on mono- or polycrystalline silicon wafers. These wafers are produced in expensive vacuum based and/or high temperature processes with large percentages of cutoff (up to 50%). An alternative is given by solution-processed film formation with silicon particles. The particles can be produced by ball milling cutoff of silicon ingots, metallurgical grade silicon or by decomposition of silane. Dispersion of silicon particles holds the possibility of simply printing a silicon film and using a roll-to-roll process to produce solar cells. The particles in the films can easily be sintered or mold together by different heat-treatments to form a percolated conducting film. Doped silicon particles of an average size of smaller than 1μm and a large size distribution are produced and used to form thin films. During handling under air atmosphere a silicon oxide shell forms on the particle surface. The silicon oxide is dissolved by treating the particles with hydrofluoric acid. The silicon particles are characterized, dispersed and spin-coated on quartz glass and silicon wafers. The films are electrically, optically and morphologically characterized and optimized. Annealing up to high temperatures leads to coalescence, sintering and melting of the film. The temperature dependent properties of the film are presented. The applications for pn-junctions and solar cells are discussed.

HL 72.5 Wed 16:00 Poster D

Structural, electronic and optical properties of random-pyramid textured Silicon wafers — •Jan Kegel[1], Heike Angermann[2], Abdelazize Laades[3], Uta Stürzebecher[3], and Bert Stegemann[1] — [1]University of Applied Sciences (HTW) Berlin, Wilhelminenhofstr. 75a, 12459 Berlin — [2]Helmholtz-Zentrum für Materialien und Energie Berlin, Kekuléstr. 5, 12489 Berlin — [3]CiS Institut für Mikrosensorik und Photovoltaik, Konrad-Zuse-Str. 14, 99099 Erfurt

In high-efficiency crystalline silicon solar cells, the surfaces of the Si wafers can be textured to reduce reflection losses and to increase the absorption probability by light trapping. This texturing is produced by anisotropic wet-chemical etching of random pyramid structures. The improvement of the optical properties, however, is associated with a larger effective surface area, which inherently corresponds to an increased number of electrically active defect states in the band gap. In this paper, a detailed, quantitative analysis of the micro-roughness of the textured Si wafers was performed. Subsequent surface conditioning was optimized with respect to efficient interface passivation as elucidated by surface photovoltage (SPV) measurements. Data on surface morphology is correlated to light-trapping behavior and interface state densities in order to identify Si wafer pre-treatment conditions for optimal solar cell performance.

HL 72.6 Wed 16:00 Poster D

Novel multifunctional emitters for heterojunction solar cells — •Henriette Gatz, Oumkelthoum Mint Moustapha, Dieuwertje Schrijvers, Bart Sasbrink, Arjen de Waal, Jatin Rath, and Ruud Schropp — Nanophotonics - Physics of Devices, Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands

Silicon heterojunctions are a promising approach to obtain high efficiency solar cells at low manufacturing costs. Their main parts consist of a silicon wafer, a thin emitter layer, and a Transparent Conductive Oxide (TCO) layer. The purpose of the TCO layer is to act as a perfect window for the incoming light while providing sufficient conductivity to transport the current to the front contact of the cell. The commonly used TCOs have several disadvantages, such as a narrow range of refractive index and work function. This does not allow for tuning in order to optimize the collection and transport of carriers.

To simplify the heterojunction silicon cell structure and its fabrication process, we aim to develop a novel layer that can be made with a

single deposition technique, combining the functions of the thin emitter layer and the TCO layer, including the anti-reflection function.

HL 72.7 Wed 16:00 Poster D

Synthesis and Characterization of Kesterite Nanoparticles and Thin Films with XRD and GDOES — •Folker Zutz, Christine Chory, Martin Knipper, Ingo Riedel, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg, Germany

Cu_2ZnSnS_4 (CZTS) is a promising compound semiconductor for low cost solar cells, because of its non-toxic and abundant precursor elements. An approach for economic manufacturing is an ink-based thin film deposition process. The inks are made from dispersions of CZTS nanoparticles, which were prepared by colloidal synthesis at low temperatures. The thin films were realized by drop casting and treated by a post-deposition annealing in inert gas atmosphere in order to remove organic stabilizers from the film and to enhance growth of polycrystalline structures. Structural investigations of dried CZTS powders with varying chemical compositions at different annealing temperatures were performed via X-ray diffraction. The development of the Kesterite phase and secondary impurity phases was investigated in order to archive a more pure CZTS material. The element distribution in the CZTS thin films was investigated by glow discharge optical emission spectroscopy (GDOES). By this method the CZTS elements and also organic compounds like precursors used during synthesis or high-boiling solvents used for the nano-ink formulation were probed. Thus the effectiveness of the NP purification and the film annealing can be analyzed.

HL 72.8 Wed 16:00 Poster D

First-principles electronic structure of β-$FeSi_2$ and FeS_2 surfaces — •Pengxiang Xu, Timo Schena, Stefan Blügel, and Gustav Bihlmayer — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Applying density functional theory in the framework of the full potential linearized augmented plane-wave (FLAPW) method FLEUR [1], we investigate the electronic structure of potential future photovoltaic materials, β-$FeSi_2$ and FeS_2, for selected surface orientations and terminations. Surface passivation has become an essential factor for translating high-efficiency solar cell concepts into industrial production schemes due to trapping of charge carriers in surface states at the passivated surface layer.

We study the atomic and electronic structure of β-$FeSi_2$ and FeS_2 thin films for (001) and (100) orientations with different terminations. The most stable orientations are determined by comparing their cohesive energy. Detailed electronic structure calculations show that surface states originating from Fe play an important role and might determine their photovoltaic properties. The effects of passivation on the electronic structure are also presented.

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[1] www.flapw.de

HL 72.9 Wed 16:00 Poster D

Optoelectronic properties of thin film Cu_2S — •Hendrik Sträter[1], Rudolf Brüggemann[1], Gottfried H Bauer[1], Sebastian Siol[2], Andreas Klein[2], and Wolfram Jaegermann[2] — [1]Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg — [2]Material- und Geowissenschaften, FG Oberflächenforschung, TU Darmstadt, D-64287 Darmstadt

Cuprous sulfide (Cu_2S) is a non-toxic and low-cost p-type semiconductor and therefore considered as an alternative for CdTe or $CuIn_xGa_{1-x}(S,Se)_2$ thin film solar cells. We investigated Cu_2S absorber layers prepared by physical vapor deposition (PVD) with varying pre- and post-treatment processes of the substrate and the Cu_2S absorber. Calibrated photoluminescence experiments with lateral μm and mm resolution were performed to obtain the splitting of the quasi-Fermi levels (QFL) μ, the absorption coefficient α and the optical band gap E_G. Additionally we have determined the local variation of the QFL-splitting across the absorber. The best sample has been prepared with both pre- and post-treatment by annealing and has a QFL-splitting of $\mu \approx 720\,\mathrm{meV}$. All samples show an optical band gap of $E_G \approx 1.3\,\mathrm{eV}$.

HL 72.10 Wed 16:00 Poster D

Cyclic voltammetry of semiconductor nanoparticles and organic materials for solar cells — •Dorothea Scheunemann, Marta Kruszynska, Joanna Kolny-Olesiak, Holger Borchert, and Jürgen Parisi — Univ. of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg

In hybrid solar cells the charge transfer between nanoparticles and conducting polymers at the donor/acceptor interface is influenced by the position of energy levels of donor and acceptor. Thus for the development of efficient solar cells it is crucial to be able to determine and control the band gap and band edge positions of donor and acceptor materials. In particular the absolute position of HOMO and LUMO levels are important. Because these band edge positions are in case of nanoparticles size-dependent, a method to estimate these positions and to relate them to the energy levels of conducting polymers is needed. One suitable method to characterize those materials is cyclic voltammetry. With this electrochemical method it is possible to detect the absolute values of the energetic positions of the HOMO and LUMO as well as non-radiative defect states with respect to the vacuum level. We present cyclic voltammetric measurements of $CuInS_2$ and ZnO nanoparticles which can be used as an acceptor material in hybrid solar cells. In addition measurements on poly(3-hexylthiophene) (P3HT) and Phenyl-C61-butyric acid methyl ester (PCBM) were done to provide electronic structures of relevant materials for hybrid as well as for organic solar cells. The measurements were done on thin films processed from solution by spin-coating.

HL 72.11 Wed 16:00 Poster D

Herstellung und Charakterisierung von Mikro-GaAs-Photovoltaikzellen — •Michael Kwiatek, Arne Ludwig, Dirk Reuter, Rüdiger Schott und Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Deutschland

In der Informationstechnologie spielen optische Übertragungswege eine immer wichtigere Rolle. So können Daten über größere Distanzen mit höherer Bandbreite übertragen werden. Ein Problem ist hierbei jedoch die Energieversorgung der angeschlossenen Endgeräte. Photovoltaik spielt bei der dezentralen Energieversorgung von Systemen eine zunehmend bedeutendere Rolle. Durch die hergestellten Mikro-Solarzellen soll diese Idee auch auf die optische Datenübertragung erweitert werden. Dem eigentlichen optischen Datensignal kann dabei eine kontinuierliche Licht-Energieversorgung überlagert werden. In diesem Beitrag wird die Umsetzung dieses Konzeptes mit Mikro-Photovoltaikzellen auf GaAs-Basis demonstriert. Es wurden auf n-Si-dotiertem GaAs-Substrat mit Molekularstrahl-Epitaxie n-p/n-i-p-Strukturen aufgewachsen. Die p-Dotierung erfolgte dabei mit einer mit Elektronen-Bombardement geheizten Kohlenstoff-Zelle. Es werden Ergebnisse mehrerer Wachstumsreihen vorgestellt, in denen die Schichtstruktur angepasst wurde, um die Charakteristik des Bauelementes zu verbessern und die Einflüsse der verschiedenen Schichtparameter zu untersuchen. Die Ergebnisse zeigen, dass die technische Umsetzung des oben formulierten Ziels prinzipiell möglich ist, so dass diese Experimente als Grundlage für weiterführende Arbeiten dienen können.

HL 72.12 Wed 16:00 Poster D

Silicon and Transparent Conducting Oxides: Si/ZnO and Si/In_2O_3 Interfaces from First Principles — •Benjamin Höffling[1,2] and Friedhelm Bechstedt[1,2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität,Max-Wien-Platz 1, 07743 Jena,Germany — [2]Eutropean Theoretical Spectroscopy Facility (ETSF)

The Transparent Conducting Oxides (TCOs) In_2O_3 and ZnO are routinely used as transparent electrodes in Si-based photovoltaics. Their interfaces with Si are consequently of great interest. Electronic band offsets, dangling bonds, and interface states determine the efficiency of charge-carrier separation in solar cells. Sample-preparation problems and difficulties in correctly describing the electronic properties of TCOs make the determination of these important quantities a challenging task to theoreticians and experimentalists alike. We develop a method for the construction of atomic models of heterostructural interfaces based on coincidence lattices, maximum bond saturation, and total energy minimization, which enables us to construct model geometries for the interface between Si and ZnO as well as between Si and In_2O_3. In particular we investigate the Si(001)/ZnO($20\bar{2}3$) and the Si(001)/In_2O_3(001) interface by means of density functional theory (DFT) and modern quasiparticle theory based on semilocal exchange-correlation functionals. We examine electronic band discontinuities and interface states. The influence of dangling bond passivation, strain, and charge transfer is studied by their respective influence

on the electronic density of states.

HL 72.13 Wed 16:00 Poster D

Numerical Simulation of Chalcogenide Solar Cells — •Olga Bakaeva[1], Felice Friedrich[1,2], Rainer Leihkauf[1], Thomas Unold[3], and Christian Boit[1] — [1]Berlin University of Technology, Sekr. E2, Einsteinufer 19, D-10587 Berlin — [2]PVcomB, Schwarzschildstr. 3, D-12489 Berlin — [3]Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, D-14109 Berlin

Numerical simulation is an essential method for fundamental understanding of solar cell physics and the improvement of the functionality of devices. Grain boundary effects and materials grading, that play an important role in chalcogenide solar cells, make it necessary to develop a model for 2D simulations. In this study, our aim was to compare the well-known one-dimensional simulation tool SCAPS1D with the commercial simulation program Sentaurus TCAD that allows for multidimensional simulation. A model with the same parameter set for Cu(In,Ga)Se2 solar cell was set up in TCAD and SCAPS1D. The effects of band alignment and generation rate on the dark and illuminated I-V characteristics were analyzed. First results of the effects of a Ga-grading in the solar cells will be discussed.

HL 72.14 Wed 16:00 Poster D

Comparative characterisation of sputtered ZnO:Al TCO-layers on float glass produced by large ceramic and metallic — •Sebastian Wohner[1], Hartmut Witte[1], Martin Bähr[2], Jörg Günther[2], Jürgen Bläsing[1], and Alois Krost[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg — [2]Euroglas GmbH, Haldensleben

One of the main parts of photovoltaic cells is the conductive and transparent front contact which is often realized by wide bandgap ZnO. D.c. magnetron sputtering with ceramic $ZnO{:}Al_2O_3$ targets is one of the commonly used processes to produce ZnO-layers on float glass. Disadvantages are the fixed stoichiometric proportions and the high temperatures.
Alternatively, Al-doped ZnO-layers were deposited by reactive d.c. magnetron sputtering from a large, planar Zn(Al) under oxygen ambience. Hereby the operating point has to be within the unstable transition region of the power - oxygen pressure characteristic.
For comparison ZnO layers were produced by reactive and by ceramic magnetron d.c. sputtering using large targets. The ZnO layers were characterized and compared by resistivity, Hall-effect as well as by optical transmission- and reflection measurements to get the electron concentration using the Drude-model. The surface and the crystal structure were analysed by AFM and Bragg-Brentano X-ray diffraction, respectively. The results show the potential for the production of qualitatively good ZnO-layers as TCO by reactive d.c. magnetron sputtering on large cathodes using adapted process controlling.

HL 72.15 Wed 16:00 Poster D

Main direction of photoelectric converters research in Georgia — •Ia Trapaidze[1], Raphiel Chikovani[1], Gela Goderzishvili[1], and Lia Trapaidze[2] — [1]Dep.of physics,Georgian Technical University,77 kostava,Tbilisi,Georgia — [2]Dep. of physics,Tbilisi State University, Chavchavadze 3,0128,Tbilisi,Georgia

Georgia together with use of traditional energy resources attaches a very large importance of using renewable energy sources. Solar energy perspective for Georgia, because of its geographical allocation on the territory and application of solar energy is an important term for providing the population with the objects which are so important for life (supply with the energy the mountainous regions of small numbers of population).In most regions of the country there are 250-280 sunny days in a year, which is approximately 1900-2000 hours per year. The prospects of development of photovoltaics in Georgia are analyzed. It is noted that the photoelectric method of conversion of the solar energy based on semiconductor materials is especially promising. Main directions of research photoelectric convertors in Georgia are: *Creation and use law power photoelectric convertors on the based of Silicon. *Processing of convertors on the base of GaAlAs and other semiconductive compounds. At present is very important to obtain high efficiency photoelectric convertors on the based of these compounds with quantum dots and quantum wells creating in nanostructure. -*Research of possibility of creation high efficiency photoelectric convertors by using silicon-germanium.

HL 72.16 Wed 16:00 Poster D

Developing coarse-grained force-fields for semiconducting polymers — •Sergii Donets, Anton Pershin, and Stephan A. Baeurle — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040 Regensburg

Semiconducting polymers have been extensively studied in the past few years due to their great potential in the solar-cell technology. Typical polymer solar cells are composed of a p-type layer for hole transport and an n-type layer for electron transport. Their perfomance is strongly dependent on the bulk heterojunction morphology, which consists of an interpenetrating network of donor and acceptor phases. In this regard computer simulation techniques can represent a powerful tool to optimize the relationship between their structural characteristics and their photovoltaic efficiency. To cope with large system sizes and lengthy equilibration times, we make use in this work of coarse-graining (CG) procedures, in which the many-particle system described at atomistic resolution is mapped onto a similar system with smaller number of degrees of freedom. To derive a suitable force-field, we use the iterative Boltzmann inversion method by iteratively refining the interaction between CG-beads, until the reference structural distributions are reproduced.

HL 72.17 Wed 16:00 Poster D

Theoretical investigation of the charge transport in nanostructured organic semiconductors — •Anton Pershin, Sergii Donets, and Stephan A. Baeurle — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040 Regensburg, Germany

Charge transport in organic semiconductors is strongly affected by small-scale loss phenomena, like exciton and charge carrier loss, which reduces the usefulness of such materials for industrial applications. In this presentation we introduce a new simulation approach, which permits to explore the causes for the occurrence of such phenomena on the nanoscale, and provide in this way a new tool for the optimization of charge transport in photovoltaic systems. Our approach models the elementary photovoltaic processes by coupling a mesoscopic simulation technique for reproducing the polymeric phase separation process with a suitable stochastic dynamical algorithm for simulating the charge transport process [1]. Using this method, we study the influence of the composition and timely variable structural factors, like e.g. inhomogeneities, on the efficiency of exciton and charge carrier generation as well as transport in nanostructured polymer systems.

[1] A. Pershin, S. Donets, S.A. Baeurle, submitted.

HL 72.18 Wed 16:00 Poster D

Characterization of hybrid solar cells based on conjugated polymers and $CuInS_2$ nanoparticles with different organic ligands — •Rany Miranti, Nikolay Radychev, Marta Kruszynska, Dorothea Scheunemann, Joanna Kolny-Olesiak, Holger Borchert, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky-Str, 9-11, 26129 Oldenburg, Germany

The performance of hybrid solar cells demonstrated considerable advances in recent years, especially concerning hybrid blends containing semiconductor nanocrystals of CdS, ZnO, or CdSe. However, materials based on cadmium chalcogenides are highly toxic which severely restricts possible applications. Moreover these materials demonstrate a relatively low absorption coefficient and the band gap of these intensively used semiconductor nanocrystals does not match the solar spectrum well. One of the promising alternative materials is the direct band gap semiconductor $CuInS_2$ (CIS). CIS absorbs up to 820 nm (Eg=1.5eV), is less toxic, and has a high absorption coefficient of about 5×10^5 cm^{-1} (at 500 nm). In the present work, CIS nanoparticles with different shapes were blended with two different kinds of conjugated polymers, namely P3HT and poly[2,1,3-benzothiadiazole-4,7-diyl[4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2,6-diyl]] (PCPDTBT). Corresponding solar cells were prepared and studied by current-voltage profiling and measurements of the external quantum efficiency. Furthermore, the influence of various organic capping ligands on the CIS-based hybrid solar cells was investigated.

HL 72.19 Wed 16:00 Poster D

Hybrid solar cells based on ZnO nanorod arrays/ polymer — •Basudev Pradhan and Dieter Neher — Institut für Physik und Astronomie, Universität Potsdam, Potsdam-Golm, Germany

Hybrid solar cells have been fabricated using vertically oriented, high density, and crystalline array of zinc oxide (ZnO) nanorods and low

bandgap hole conducting polymer. These hybrid solar cells take advantage of the both materials properties: solution processing of polymers and high electron mobility of inorganic semiconductors. The vertical nanorods provide direct conduction paths for the electrons from the point of injection to the collection electrode while maintaining large interface area between polymer and nanorod arrays. We have found that the device performance improves with deep infiltration of the polymer into the nanorod arrays and also with the improved crystallinity of the polymer induced by post annealing. In addition, the dependence of photovoltaic performance on the ZnO nanorod length was investigated and different low bandgap polymers have been used to achieve optimum performance.

HL 72.20 Wed 16:00 Poster D

Growth and characterization of sublimation grown 9,10-diphenylanthracene single crystals — •T. Schmeiler[1], M. Zellmeier[1], and J. Pflaum[1,2] — [1]Exp. Phys. VI, Julius-Maximilians-University Würzburg, D-97074 Würzburg — [2]ZAE Bayern e.V. , D-97074 Würzburg

Organic single crystals define an important class of solid states due to their structural, chemical and functional homogeneity. In case of polyaromatics, single crystals provide reference systems with respect to optical properties, charge carrier transport and their respective spatial anisotropies. Here we present a study on 9,10-diphenylanthracene (DPA) single crystals grown via sublimation under streaming nitrogen gas. The lateral extension of the DPA crystal reveals (010) facet areas up to 0,5 cm^2 at thicknesses of 100 μm. The high structural quality is confirmed by X-ray diffraction as well as by the charge carrier transport measured by time-of-flight (TOF). To map existing dislocation lines, we developed an etching protocol which, as for the case of 5,6,11,12-tetraphenyltetracene (rubrene), yields to pyramidal-shaped etch pits at termination points of the [001] dislocation lines. Depending on etching conditions, like concentration and time, the sizes of the epitaxially oriented pits can be tuned in the range of several micrometres thereby promising interference with optical excitation wavelenght. In the case of rubrene, such structures were already investigated by means of Photoluminescence (PL) measurements in combination with FDTD simulations, both revealing enhanced PL-intensities at the pit edges due to waveguiding and enhanced light scattering.

HL 72.21 Wed 16:00 Poster D

Investigation of recombination processes in organic solar cells using a differential photocurrent method. — •Simon Hein[1], Julia Rauh[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg

To satisfy the world's need for energy organic solar cells offer, due to their low fabrication costs, a promising alternative. Although power conversion efficiencies of 9.2 % have already been achieved on lab scale [1], the fundamental processes taking place in organic solar cells are still not completely understood. One of the currently most discussed topics is the dominating recombination process of charge carriers, as this loss mechanism influences all of the relevant solar cell parameters. Therefor, a detailed understanding of the recombination mechanisms is essential for further efficiency enhancement. Recently, Koster et al. [2] presented a technique to investigate the influence of light intensity on the charge carrier recombination under short-circuit conditions. Thereby, the differential current density, induced by a modulated light of low intensity superimposed to a continuous background light of various intensities, is measured. We present our data obtained by this technique for poly(3-hexylthiophene) solar cells blended with different electron acceptors. The results are discussed with respect to the charge carrier recombination processes under short-circuit conditions in dependence of temperature and a wide range of light intensities.

[1] R. F. Service, Science, 332, 293 (2011)
[2] L. J. A. Koster et al., Adv. Mater., 23, 1670 (2011)

HL 72.22 Wed 16:00 Poster D

Recombination of excited species in organic photovoltaic material systems studied by field dependend transient absorption — •Clemens Grünewald[1], Julia Kern[1], Julien Gorenflot[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg

Organic opto-electronic devices such as bulk heterojunction solar cells are limited in their efficiency due to intrinsic geminate and non-geminate charge carrier losses. The recombination dynamics of the latter mechanism are observed with time resolved photoinduced absorption spectroscopy from submicro- to milliseconds at different temperatures and wavelengths to address polarons. Starting with the well-probed poly(3-hexylthiophene) : [6,6]-phenyl-C61-butyric acid methyl ester (P3HT:PCBM) material system the study also covers promising donor polymers such as PTB7. In addition an external electric field is applied to these organic blends in order to address charge carrier generation and recombination behaviour under bias. The dependence of the photogeneration of free charge carrier on electric field and temperature are described in relation to the Braun-Onsager model.

HL 72.23 Wed 16:00 Poster D

Transient resolved recombination measurements in organic bulk heterojunction solar cells — •Markus Gluecker[1], Alexander Foertig[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg, Germany — [2]Bavarian Centre for Applied Energy Research (ZAE Bayern e.V.), Am Hubland, 97074 Würzburg, Germany

The understanding of the current–voltage behavior is a prerequisite for improving the solar cell performance. Transient photovoltage (TPV), transient photocurrent (TPC) and voltage dependent charge extraction (CE) measurements were applied to organic solar cells based on different polymer:fullerene blend systems. From the determined charge carrier decay mechanism under open circuit conditions and voltage dependent charge carrier densities $n(V)$ the measured I/V response can be reconstructed. For material systems such as poly(3-hexyl thiophene)(P3HT):[6,6]-phenyl-C_{61} butyric acid methyl ester (PCBM) characterized by a voltage independent charge generation, we verified that bimolecular recombination is sufficient to describe the I/V behaviour over the entire operational regime. We further address the temperature dependent applicability of this analysis.

HL 72.24 Wed 16:00 Poster D

Optical properties of single crystalline pentacene and perfluoropentacene layers — •Jonatan Helzel, Mathias Schulz, Mira El Helou, Tobias Breuer, Gregor Witte, and Wolfram Heimbrodt — Philipps Universität Marburg department of physics and material sciences centre Germany, Renthof 5, D-35032 Marburg

We prepared pentacene films with thicknesses of 10 nm, 20 nm and 100 nm on different ZnO surfaces by molecular beam deposition under ultra-high vacuum conditions. By varying the growth temperature, we prepared pentacene films in an amorphous phase, in the thin film phase and the Campbell phase. To characterize the films AFM and X-ray diffraction measurements have been done. The pentacene molecules form single crystalline islands with extensions of several μm. So we were able to measure the absorption on single islands and found a polarisation dependence of both Davydov components perpendicularly to each other. The electronic transitions of the pentacene films have been measured in the temperature range between 10 K and room temperature. We observed a thickness dependent shift of the pentacene states upon cooling. At 10 K there is a difference of about 30 meV between the electronic states of a 10 nm and a 100 nm thick pentacene film. The reason for this behaviour is the very different thermal expansion coefficients of substrate and film resulting in a strong in-plane tensile strain. This strain causes little rifts in the film, which leads to a hysteretic temperature shift of the excitons. Analogous measurements have been done on single crystalline perfluoropentacene on KCl and NaF substrates.

HL 72.25 Wed 16:00 Poster D

Organic semiconducting complexes at the molecular scale — •Matthieu Dvorak, Markus Müller, Frank Stienkemeier, and Elizabeth von Hauff — Physics Institute, University of Freiburg, Hermann-Herder Str. 3, 79104 Freiburg, Germany

An improved understanding of the parameters which influence the charge transfer between donor and acceptor molecules is highly important to improve the efficiency of organic solar cells. Different parameters such as the bulk mobility, the molecular structure and the ordering proved to play an important role on the charge transfer.[1] In thin film or solution systems it is most of the time not possible to disentangle these different mechanisms at a molecular scale. On the contrary, helium droplets, due to their cold, superfluid and weak interacting properties, has proved to be the perfect matrix for the study of optical properties at the molecular scale, related to a spectral resolution increased by three orders of magnitude compared to thin film or solution measurements. This precision proved to be helpful to

confirm recent calculations on PTCDA complexes (3,4,9,10-perylene-tetracarboxylic- dianhydride) based on a Frenkel exciton model.[2]
Making use of the enhanced spectroscopic resolution to study the charge transfer process at a molecular scale as well as the possibility to vary the donor-acceptor distance are expected to reveal new information to improve the charge transfer in donor-acceptor systems which is relevant in organic photovoltaic.

[1] M. Hallermann *et al.*; Appl. Phys. Lett., 97, 023301 (2010)
[2] J. Roden *et al.*; J. Chem. Phys., 134, 054907 (2011)

HL 72.26 Wed 16:00 Poster D

Charge transport in organic semiconductors - electric potential mapping — •Johannes Widmer, Wolfgang Tress, Karl Leo, and Moritz Riede — Institute für Angewandte Photophysik, TU Dresden, Germany

The charge transport in thin films of organic semiconductors is characterized in single carrier devices of small molecule organic semiconductors. We observe space-charge limited currents (SCLC) in devices with varying layer thicknesses. This enables us to determine the electric field evolution within the material, i.e. we can characterize the charge current in more detail than in individual space-charge limited devices.

Single carrier devices allow for the characterization of current in the same geometry as in typical applications (in contrast to field effect transistors) and with adequate parameters: The current density, the electric field, as well as the charge carrier density in these measurements have similar values as in e.g. organic solar cells or OLEDs.

The presented evaluation method is an extension of single SCLC measurements and can give insight into device-relevant details of the charge transport.

HL 72.27 Wed 16:00 Poster D

Bottom-gated test bed for organic field-effect transistors with epitaxial graphene electrodes — •Emmanuel Bayaya, Daniel Waldmann, Johannes Schöck, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7 / Bau A3, 91058 Erlangen

We fabricate organic field-effect transistors with graphene source- and drain electrodes, using epitaxial graphene on silicon carbide (0001).A bottom-gate is provided by implantation prior to graphene growth [1]. This setup provides an ultra flat test bed for organic semiconductors, or other materials. We demonstrate gate operation for Poly(3-hexylthiophene), and critically discuss the role of interface states being created during the fabrication.

[1] D. Waldmann, J. Jobst, F. Speck, T. Seyller. M. Krieger, H.B. Weber, Nature Materials 10, 357-360 (2011).

HL 72.28 Wed 16:00 Poster D

Quantitative Kelvin probe force microscopy investigations of organic field-effect transistor channels — •Jan Murawski, Peter Milde, Moritz P. Hein, Merve Anderson, and Lukas Eng — TU Dresden, Institut für Angewandte Photophysik, George-Bähr-Str. 1, 01069 Dresden

Organic field-effect transistors (OFETs) are popular for several decades by now. Although expected to have a great impact on semiconductor electronics in the near future, OFETs still suffer from drawbacks such as high injection and extraction barriers at the electrodes and low charge carrier mobilities. Typically, only macroscopic values for these parameters are obtained, while the microscopic origins remain unknown.

In this contribution, we investigate channels of pentacene and poly[9,9-dio-ctyl-fluorene-co-N-(4-butylphenyl)-diphenylamine] (TFB) based bottom-gate, bottom-contact OFETs using non-contact atomic force microscopy (nc-AFM) combined with frequency-modulated Kelvin probe force microscopy (FM-KPFM) [1] for mapping the surface potential with high sensitivity in ambient conditions. With this method we are able to visualize the local injection and extraction barriers, quantify their heights, and discover bottlenecks of charge transport within these devices.

[1] U. Zerweck et al., Accuracy and Resolution Limits of Kelvin Probe Force Microscopy. Phys. Rev. B 71:125424 (2005)

HL 72.29 Wed 16:00 Poster D

Charge Transport in organic solar cells studied by Scanning Probe Microscopy — •Michael Scherer[1,2], Dominik Daume[1,2], Rebecca Saive[1,2], Daniela Donhauser[1,3], Michael Kroeger[1,3], Irene Wacker[4], Rasmus Schröder[1,5], and Wolfgang Kowalsky[1,3] — [1]Innovation Lab GmbH — [2]Universität Heidelberg — [3]Technische Universität Braunschweig — [4]Institut für Biologische Grenzflächen, Karlsruher Institut für Technologie — [5]CellNetworks, BioQuant, Universität Heidelberg

We report on the characterization of P3HT:PCBM bulk heterojunction organic solar cells via scanning probe microscopy. We fabricated OPV devices on various substrates to then prepare thin lamellas via micro-cutting techniques to allow for SPM characterization of device cross-sections.

HL 72.30 Wed 16:00 Poster D

Toward the realization of a Scanning Near-field Optical Microscope deploying an Organic Light Emitting Device — Ilja Vladimirov[1,2], •Benjamin Martini[1,4], Daniela Donhauser[1,3], Johannes Ostermann[1,3], Michael Kröger[1,3], and Wolfgang Kowalsky[1,3] — [1]Innovation Lab, Heidelberg — [2]Universität Heidelberg, Kirchhoff-Institut für Physik — [3]TU Braunschweig, Institut für Hochfrequenztechnik — [4]TU München

We investigate a scanning near-field optical microscope (SNOM) employing an organic light emitting device (OLED) fabricated on a commercial atomic force microscope (AFM) cantilever via vacuum thermal evaporation and a method for its characterization. In order to deposit the OLED on a silicon cantilever, the OLED stack based on transparent ITO anode was adapted to silicon, the direction of light emission inverted and the out-coupling efficiency optimized. Employment of luminescent dopants led to OLED luminance values on silicon of about 1000 cd/m^2 at 7 V.
Due to the low photon flux, estimated to be below 1000 photons/second, we use a photon counter, based on a cooled photomultiplier (PMT) to detect photons emitted from the AFM tip. To verify the applicability of near-field condition, we use a tapered optical fiber featuring a distribution of propagating modes significantly beyond the fiber core. This allows to detect coupling between the evanescent near-field of the probe and the modes of the tapered fiber using the PMT. Distance control between tip and sample is accomplished by an AFM.

HL 72.31 Wed 16:00 Poster D

Exploring molecular-scale structure formation of HIOS by all-atom Molecular Dynamics computer simulations — •Karol Palczynski and Joachim Dzubiella — Helmholtz-Zentrum Berlin, Hahn Meitner Platz 1, 14109 Berlin

The optical and electronic properties of Hybrid Inorganic/Organic Semiconductor (HIOS) devices strongly depend on the molecular configuration of the conjugated organic molecules (COM) at the inorganic semiconductor surfaces. The goal of this work is to explore the structure formation of HIOS on a molecular level by applying atomistically resolved molecular dynamics (MD) computer simulations of various COM. The temperature dependent crystal structures of COM such as Diindenoperylene, P-Sexiphenyl and Coronene have been investigated with various MD simulation methods. The sensitivity of the obtained structures to atomic partial charges and charge distributions has been studied. The calculated results have been compared with experimental x-ray measurements. Interaction parameters suitable for coarse-graining simulations have been determined.

HL 72.32 Wed 16:00 Poster D

Influence of charge carrier density and dimensionality on transport properties of (DCNQI-d$_6$)$_2$Cu radical anion salts — •Florian Hüwe[1], Matthias Schmiddunser[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University Würzburg, D-97074 Würzburg — [2]ZAE Bayern e.V., D-97074 Würzburg

Due to their quasi-1D band structure the highly conducting organic (DCNQI-d$_6$)$_2$Cu radical anion salts provide an insight into the physics of low-dimensional metals. Compared to ordinary 3D metals they undergo a first-order Peierls metal-insulator transition upon cooling and show much more pronounced interactions with electrons and phonons.

Our contribution reports on the electrocrystallization of needle-like (DCNQI)$_2$Cu single crystals with extensions of up to $3cm$ along the (001) direction of high conductivity and thicknesses up to $125\mu m$ along the (010) normal. Characterization by XRD, Raman spectroscopy and transport measurements confirms the high quality of the samples. Their room-temperature conductivities reach values up to $\sigma = 1200 Scm^{-1}$ and show Ohmic behaviour. Raman spectra indicate an increase in charge carrier density on the crystallized DCNQI molecules compared to the neutral molecules causing partial filling of

the conduction band. Upon cooling the $(DCNQI)_2Cu$ crystal undergo a characteristic Peierls transition at $T_p = 75K$. To further elucidate effects by size and carrier concentration, these results will be compared to sub-μm sized crystallites smaller than $5\mu m$ and to crystals with modified charge carrier densities.