

HL 90: Poster III

Topics: Organic-inorganic perovskite semiconductors, Graphene, Oxide Semiconductors other than ZnO, Organic photovoltaics and electronics, Quantum information systems, Carbon: Diamond, nanotubes

Time: Thursday 16:00–19:00

Location: Poster A

HL 90.1 Thu 16:00 Poster A

In Situ Raman Spectroscopy for the Characterization of Plasma Textured Black Silicon — •MARIA GAUDIG^{1,2}, JENS HIRSCH^{1,3}, DOMINIK LAUSCH³, PAUL-T. MICLEA^{2,3}, ALEXANDER N. SPRAFKE², NORBERT BERNHARD^{1,3}, and RALF B. WEHRSPORN^{2,4} — ¹Anhalt University of Applied Sciences, Technologies of Photovoltaics Group, Bernburger Str. 55, D-06366 Köthen — ²Martin Luther University Halle-Wittenberg, Institute of Physics, Group mikroMD, Heinrich-Damerow-Str. 4, D-06120 Halle (Saale) — ³Fraunhofer Center for Silicon Photovoltaics CSP, Otto-Eißfeldt-Straße 12, D-06120 Halle (Saale) — ⁴Fraunhofer Institute for Mechanics of Materials IWM, Walter-Hülse-Str. 1, D-06120 Halle (Saale)

Black silicon (b-Si) promises with its extremely low reflectivity to become a real alternative to wet chemical textured silicon in the PV industry. In this work, the nano texturing is realized with a maskless SF₆/O₂ plasma etch process. We showed different plasma textures with absorption about 95 % and effective lifetimes in the microsecond, which is adequate for solar cells. However, the physical understanding behind the b-Si formation is still insufficient. To clarify the creation of these small nano-needles by a maskless process, we applied Raman spectroscopy, which provides information about the surface roughness, stress or amorphous silicon formation and the chemical composition on the surface. A Raman probe is constructed inside the plasma etch chamber. Transient Raman spectra were measured and evaluated. In this contribution, we will show the results of these in situ measurements and our conclusions concerning the b-Si formation.

HL 90.2 Thu 16:00 Poster A

Improved Selenization Process of Wet-Chemically Fabricated Cu₂ZnSn(S,Se)₄ Absorbers for Thin-Film Solar Cells — •MARKUS NEUWIRTH¹, HUIJUAN ZHOU¹, MARIO LANG¹, NIKLAS MATHES¹, THOMAS SCHNABEL², ERIK AHLWEDE², MICHAEL POWALLA^{2,3}, HEINZ KALT¹, and MICHAEL HETTERICH¹ — ¹Institute of Applied Physics, Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart — ³Light Technology Institute, Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe

Solar cells based on Cu₂ZnSn(S,Se)₄ (CZTSSe) are promising since they only comprise environmentally friendly and earth-abundant elements. However, their conversion efficiency is still too low to be competitive and especially good reproducibility of high-efficiency devices is a major issue. Our fabrication approach for CZTSSe consists of a cheap and simple solution-based process that spares toxic solvents such as hydrazine. Optimizing the selenization process of the doctor-bladed precursors led to a significantly improved reproducibility and energy conversion efficiencies of up to 7

HL 90.3 Thu 16:00 Poster A

Kelvin Probe Force Microscopy Studies of CIGS Solar Cells — •JASMIN SEEGER¹, ZHENHAO ZHANG^{2,4}, WOLFRAM WITTE³, MICHAEL POWALLA^{2,3}, HEINZ KALT¹, and MICHAEL HETTERICH¹ — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ²Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ³Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany — ⁴Present address: Singulus Technologies AG, 63796 Kahl am Main, Germany

Cu(In,Ga)Se₂ (CIGS) is a well-established absorber material for thin-film solar cells, achieving conversion efficiencies of up to 21.7%. In order to further improve this performance, a detailed understanding of the potential distribution (width of the space charge region etc.) in these devices is essential. Of particular interest are the impact of alternative buffer materials or a variation of the gallium content of the absorber on the device performance. To study this impact we investigate the surface as well as the cleaved edge of CIGS solar cells utilizing Kelvin Probe Force Microscopy (KPFM). The contact potential difference (CPD) is studied through the complete structure, partly even on illuminated operating devices. The results are correlated with complementary data such as I-V characteristics and give insights into

loss mechanisms in CIGS solar cells.

HL 90.4 Thu 16:00 Poster A

Time-resolved photoluminescence in Cu₂ZnSn(S,Se)₄ solar cells — •MARIO LANG¹, ALEXANDER OPOLKA¹, CHRISTOPH KRÄMMER¹, TOBIAS ABZIEHER², THOMAS SCHNABEL², ERIK AHLWEDE², MICHAEL POWALLA^{2,3}, HEINZ KALT¹, and MICHAEL HETTERICH¹ — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany — ³Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Solar cells made of Cu₂ZnSn(S,Se)₄ (CZTSSe) offer a high potential for commercial application. So far efficiencies up to 12.6% have been achieved, but the material suffers from its high open-circuit voltage deficit. The origin of this huge deficit is still an open question, but can probably be attributed to the complex defect structure of the material. Spectrally as well as time-resolved photoluminescence (TRPL) are suitable methods to gain information about the defect structure and can be used to further study the physical recombination mechanisms in CZTSSe solar cells. In this contribution we investigate the decay dynamics and loss mechanisms by time-resolved photoluminescence in dependence of excitation power and temperature.

HL 90.5 Thu 16:00 Poster A

State-Filling Versus Screening of Electrostatic Potential Fluctuations in Cu₂ZnSn(S,Se)₄ thin-film solar cells — CHRISTIAN ZIMMERMANN¹, CHRISTOPH KRÄMMER¹, MARIO LANG¹, •TOBIAS RENZ¹, TOBIAS ABZIEHER², THOMAS SCHNABEL², ERIK AHLWEDE², MICHAEL POWALLA^{2,3}, CHRISTIAN HUBER¹, HEINZ KALT¹, and MICHAEL HETTERICH¹ — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart — ³Light Technology Institute, KIT

Cu₂ZnSn(S,Se)₄ (CZTSSe) is a promising alternative for the well-established absorber material Cu(In,Ga)Se₂ in thin-film solar cells. However, the efficiency of CZTSSe devices is still not competitive and essentially limited by an insufficient open-circuit voltage. Excitation power-dependent photoluminescence (PL) measurements show a “blue-shift“ of the PL maximum by 15–20 meV/decade. This is often explained by a screening of electrostatic potential fluctuations caused by charged defects. In literature, electrostatic potential fluctuations are often held accountable for the low V_{OC}. In this contribution we investigate excitation-power dependent PL at 10K. We can show by analyzing the whole PL lineshape that the observed “blue-shift“ is rather dominated by filling of defect states than by a screening of electrostatic potential fluctuations.

HL 90.6 Thu 16:00 Poster A

Characterization of absorber and buffer layers in Cu₂ZnSn(S,Se)₄ solar cells by electroreflectance — •NICOLAS SCHÄFER¹, CHRISTOPH KRÄMMER¹, CHRISTIAN HUBER¹, MARIO LANG¹, TOBIAS ABZIEHER², THOMAS SCHNABEL², ERIK AHLWEDE², MICHAEL POWALLA^{2,3}, HEINZ KALT¹, and MICHAEL HETTERICH¹ — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany — ³Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Cu₂ZnSn(S,Se)₄ (CZTSSe) is a promising thin-film solar cell absorber material. One of its main advantages compared to the well-established Cu(In,Ga)Se₂ (CIGS) is the absence of expensive and environmentally problematic indium and gallium. However, especially the achieved open-circuit voltages are still a problem and the CdS buffer adopted from the CIGS device architecture may not be optimal. In our study we use electromodulated reflectance (ER) to study the band structure of both the CZTSSe absorber and buffer. In this context the impact of post-annealing procedures and the application of alternative buffer layers on the absorber/buffer interface is of particular interest.

HL 90.7 Thu 16:00 Poster A

Co-evaporation of alternative buffer layers in CZTSSe solar cells — ●MAX REIMER¹, MARKUS NEUWIRTH¹, LWITIKO MWAKYUSA¹, MICHAEL WOLFSTÄDTER^{1,2}, ERIK AHLWEDE², MICHAEL POWALLA^{2,3}, HEINZ KALT¹, and MICHAEL HETTERICH¹ — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany — ³Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

$\text{Cu}_2\text{ZnSn}(\text{S,Se})_4$ (CZTSSe) has drawn wide interest as an alternative absorber layer in thin-film solar-cells due to its composition of environmentally friendly and low-cost materials. However, CZTSSe solar cells suffer from their low open-circuit voltage and hence from a low efficiency. The solar cell structure of CZTSSe solar cells is mainly adopted from the well-established $\text{Cu}(\text{In,Ga})\text{Se}_2$ solar cells and thus CdS is typically used as buffer layer. The CdS buffer layer could be one limiting factor for the low open-circuit voltage due to a non-optimal band alignment between the buffer and the absorber. It also reduces the short-circuit current since its band gap is too small, leading to parasitic absorption. In this study we co-evaporate different II-VI semiconductors as alternative buffer layers on CZTSSe solar cells. The buffer layers are analysed concerning their capability as suitable buffer layers for CZTSSe solar cells.

HL 90.8 Thu 16:00 Poster A

Wet-Chemical Processing of CdS and Alternative Buffer Layers for $\text{Cu}_2\text{ZnSn}(\text{S,Se})_4$ Solar Cells . — ●LWITIKO MWAKYUSA¹, MARKUS NEUWIRTH¹, NIKLAS MATHES¹, MARIO LANG¹, THOMAS SCHNABEL², ERIK AHLWEDE², MICHAEL POWALLA^{2,3}, BRYCE RICHARDS^{3,4}, HEINZ KALT¹, and MICHAEL HETTERICH¹ — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany — ³Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ⁴Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), 76344 Karlsruhe, Germany

Solar cells based on $\text{Cu}_2\text{ZnSn}(\text{S,Se})_4$ (CZTSSe) are promising since they only comprise environmentally friendly and earth-abundant elements. However, their device architecture which has been adopted from $\text{Cu}(\text{In,Ga})\text{Se}_2$ (CIGS) is not yet optimal. This holds in particular for the CdS buffer. In this contribution we study the fabrication of alternative buffer layers, especially that of $(\text{Cd,Zn})\text{S}$ and their impact on the performance of CZTSSe solar cells.

HL 90.9 Thu 16:00 Poster A

X-Ray Absorption of Kesterite-Based Materials Studied from First Principles — ●ARCHANA MANOHARAN¹, LORENZO PARDINI¹, KARSTEN HANNEWALD^{1,2} und CLAUDIA DRAXL^{1,2} — ¹Humboldt-Universität zu Berlin, Institut für Physik und IRIS Adlershof, Zum Großen Windkanal 6, 12489 Berlin, Germany. — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany.

The kesterite material $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) and its Ge-substituted derivative $\text{Cu}_2\text{ZnGeS}_4$ (CZGS) are considered as good absorber material for photovoltaic applications. Here, we study the X-ray absorption spectra of CZTS and CZGS by solving the Bethe-Salpeter equation of many-body perturbation theory on top of density-functional theory. The *ab-initio* calculations are carried out using the all-electron full-potential code **exciting**. Special emphasis is put on comparative studies of the sulfur K and $L_{2,3}$ edges in CZTS and CZGS as well as in its stable binary phase ZnS. A detailed analysis and interpretation of the observed spectral signatures, in particular, the Coulomb interaction between core hole and conduction electrons is performed.

HL 90.10 Thu 16:00 Poster A

Laser-induced shockwave delamination: A non-thermal structuring method of functional thin films — ●PIERRE LORENZ¹, TOMI SMAUSZ^{2,3}, TAMAS CSIZMADIA², LUKAS BAYER¹, MARTIN EHRHARDT¹, KLAUS ZIMMER¹, and BELA HOPP² — ¹Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany — ²Department of Optics and Quantum Electronics, University of Szeged, H-6720 Szeged, Dóm tér 9, Hungary — ³MTA-SZTE Research Group on Photoacoustic Spectroscopy, University of Szeged, H-6720 Szeged, Dóm tér 9, Hungary

Shock-wave-induced film delamination (SWIFD) as non-thermal laser patterning process enables a gentle film removal and offers therefore a

great potential for application. At the SWIFD, the localized removal of the functional thin films is induced by a shock wave which is produced by a laser ablation with 25 ns and 248 nm laser pulses applied to the rear side of the substrate. Different film / substrate combination was tested e.g. copper indium gallium selenide (CIGS) solar cell stacks on polyimide and steel carrier foil and indium tin oxide (ITO) on polyethylene terephthalate (PET). The morphology and the composition of the structures were analysed by optical and scanning electron microscopy (SEM) and by energy-dispersive X-ray spectroscopy (EDX), respectively. Furthermore, the mechanism of SWIFD was analyzed by shadowgraph experiments and this will allow improvements of the physical understanding, modelling and process optimization.

HL 90.11 Thu 16:00 Poster A

Impact of gas exposure on electronic properties of methylammonium lead iodide films — ●BERND EPDING^{1,3}, CHRISTIAN MÜELLER^{1,2,3}, ROBERT LOVRINCIC^{2,3}, and WOLFGANG KOWALSKY^{1,2,3} — ¹Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — ²Institut für Hochfrequenztechnik, TU Braunschweig, Germany — ³Innovation Lab, Heidelberg, Germany

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 20%. This is even more impressive if we take into account that such high efficiencies can be reached for various cell designs, made from different precursor materials, for both solution and vacuum processed absorber layers. Even though very good devices can already be manufactured, the exact mechanisms, which lead to good charge carrier mobility and extraction, are still not fully understood.

We focus in this work on a comparison between perovskite layers (and solar cells based thereon) in different surrounding atmospheres to investigate the role of intercalated water [1]. Scanning Kelvin probe microscopy was performed under different atmospheric conditions. Thereby we are able to map electronic and structural properties with high spatial resolution. Together with IV measurements, this allows us to directly correlate the obtained data to device performance.

[1] C. Mueller et al., Chem. Mater., 2015, 27 (22), p. 7835-7841

HL 90.12 Thu 16:00 Poster A

Stabilization of $\text{CH}_3\text{NH}_3\text{PbI}_3$ in Humid Air by Partial Substitution of Iodide by Bromide — ●RAFFAEL RUESS, MARTINA STUMPP, and DERCK SCHLETTWEIN — Institute of Applied Physics, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany.

Thin films of methylammonium lead halides $\text{CH}_3\text{NH}_3\text{Pb}(\text{I}_{1-x}\text{Br}_x)_3$ were prepared onto FTO substrates and exposed to humid air in the dark. To characterize the stability of the materials, UV-vis spectra were acquired at fixed intervals, accompanied by X-ray diffraction, energy dispersive X-ray spectroscopy, scanning electron and confocal laser scanning microscopy. Two different degradation mechanisms were observed. It was confirmed that bromide slowed down the formation of PbI_2 . Furthermore, it was found that the formation of the perovskite monohydrate phase was successfully suppressed, presumably caused by stronger hydrogen bonding interactions between the organic cation and bromide ions. The use of an increased bromide content in methylammonium lead halide absorbers is discussed for the application in perovskite solar cells.

HL 90.13 Thu 16:00 Poster A

Lasing in lead iodide perovskite thin films on distributed feedback gratings — ●MAREIKE STULZ^{1,2}, PHILIPP BRENNER¹, AINA QUINTILLA¹, HOLGER RÖHM¹, IAN HOWARD³, ALEXANDER COLSMANN¹, HEINZ KALT², and ULI LEMMER¹ — ¹Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ²Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ³Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

Hybrid organic-inorganic perovskites have recently shown great potential as gain material for laser devices with the advantages of solution processability, wavelength tunability and high stability [1]. Furthermore, the low trap densities and high charge carrier mobilities might enable electrically pumped gain in this material.

We prepared thin films of Methylammonium lead iodide ($\text{CH}_3\text{NH}_3\text{PbI}_3$) on corrugated substrates by solution-based spin-coating or doctor blading. Matching the film thickness and grating period enabled optically pumped distributed feedback single mode las-

ing at room temperature. Additionally, the modal net gain of the perovskite thin films was measured with the variable stripe length method.

[1] Xing et al. Nature Materials 13, 476-480, 2014.

HL 90.14 Thu 16:00 Poster A

Radiative loss mechanisms in hybrid trihalide perovskite films — ●ROBERT HANFLAND, FABIAN MEIER, CHRISTOPH BAUMBACH, and CARSTEN DEIBEL — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

During the last few years, hybrid trihalide perovskite based solar cells showed an impressive ascent of efficiency and recently reached values beyond 18 %. Recombination mechanisms as the main loss mechanism control the dynamics of photoluminescence (PL) and play an important role for further improvement of efficiency.

We investigated the recombination mechanisms in hybrid trihalide perovskite films by using a confocal setup for PL measurement. The measured transients were analysed using models with different recombination mechanisms such as direct or trap assisted recombination. Other processes like multiple trapping are included as well. We discuss the dominant recombination mechanisms in view of its implications on the device performance.

HL 90.15 Thu 16:00 Poster A

Electronic structure of lead halide perovskite — ●DANIEL NIESNER^{1,2}, TYLER J. S. EVANS¹, BRYAN J. KUDISCH¹, PRAKRITI P. JOSHI¹, KIYOSHI MIYATA¹, XIAOXI WU¹, M. TUAN TRINH¹, HAIMING ZHU¹, MANUEL MARKS¹, and X.-Y. ZHU¹ — ¹Department of Chemistry, Columbia University, New York, NY 10027, USA — ²Festkörperphysik, FAU Erlangen-Nürnberg, D-91058 Erlangen, Germany

Angle-resolved photoelectron spectroscopy (ARPES) and two-photon photoelectron spectroscopy give insight into the valence and conduction band electronic structure of semiconductors. Doping levels can directly be extracted. Experiments require samples with well-defined surfaces. We report the preparation of high-quality polycrystalline thin films of $(\text{CH}_3\text{NH}_3)\text{PbI}_3$ on native silicon oxide on Si(111), sapphire, and PbSe(001). The (110) crystalline axis is orientated along the surface normal. Surface roughness is 1 nm. ARPES data are in semiquantitative agreement with band structure calculations. The valence band is located 1.5 ± 0.1 eV below the Fermi level E_F . The films on oxide surfaces are highly to degenerately n-doped, with the conduction band minimum up to 0.08 eV below E_F . Photoemission techniques are combined with optical spectroscopy taking into account the Burstein shift resulting from the high doping level. The band gap is 1.535 ± 0.030 eV, in good agreement with the reported value for single-crystalline $(\text{CH}_3\text{NH}_3)\text{PbI}_3$.

HL 90.16 Thu 16:00 Poster A

The influence of fabrication process and substrate material on electrical characteristics of methylammonium lead iodide — ●TIM HELDER^{1,2}, CHRISTIAN MUELLER^{1,2,3}, WOLFGANG KOWALSKY^{1,2,3}, and ROBERT LOVRINCIC^{2,3} — ¹KIP, Universität Heidelberg, Germany — ²InnovationLab, Heidelberg, Germany — ³IHF, TU Braunschweig, Germany

Research interest in halide perovskites such as $\text{CH}_3\text{NH}_3\text{PbI}_3$ as photovoltaic materials has increased continuously in the last years due to an increase of solar cell efficiencies to over 20%. This development is even more impressive if we take into account the possibilities in variation of substrates, precursor materials and fabrication methods. Despite all these efforts we still lack in understanding fundamental processes in solar cells based on these materials.

Herein we present Kelvin Probe measurements to investigate the impact of fabrication processes on the work function of $\text{CH}_3\text{NH}_3\text{PbI}_3$ layers. Therefore we deposited $\text{CH}_3\text{NH}_3\text{PbI}_3$ by spincoating and vacuum evaporation. Moreover, we varied the process parameters of single process steps (e.g. annealing) as well as the substrate materials (e.g. PEDOT, TiO_2 , Au). Thereby we are able to directly investigate the impact of single changes in the fabrication process on the electrical behavior of the perovskite layer. We will discuss implications of our results for solar cell performance.

HL 90.17 Thu 16:00 Poster A

Charge dynamics of Organometal Trihalide Perovskite using broadband transient absorption technique — ●YAJUN GAO¹, TOBIAS SCHNIER², KESTUTIS BUDZINAUSKAS¹, JINGYI ZHU¹, SELINA OLTHOFF², KLAUS MEERHOLZ², and PAUL LOOSDRECHT¹ — ¹Physics Institute II, University of Cologne, Zùlpicher street 77, 50937, Cologne,

Germany — ²Physical Chemistry, University of Cologne, Luxemburger street 116, 50939, Cologne, Germany

Organometal trihalide perovskites provide a promising alternative for photovoltaic applications, with the highest solar cell power conversion efficiency of 19.3% as reported in 2014. The precise mechanism of power conversion in these materials is currently not well understood. In this work, we address this issue using visible and near-infrared broadband transient absorption (TA) spectroscopy, which can discriminate between free charges and excitons, to study the ultrafast charge generation in organometal trihalide perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$ films. Charge selectivity is achieved by observing the transient response of charge-selective extraction layers, PCBM for electrons and spiro-OMeTAD for holes, spin-coated on the perovskite film. In addition to the response of the charge-selective layers, additional TA features show up which are attributed to free charges in the perovskite film. We use these experiments to determine the diffusion length of excitons and free carriers in the perovskite film, a property which is of central importance to the functionality of perovskite based solar cell devices.

HL 90.18 Thu 16:00 Poster A

Temperature-dependent absorption measurements and photoluminescence spectroscopy of mixed organic-inorganic halide perovskite films — ●ANGELIKA SCHULZ¹, FABIAN RUF¹, NADJA GIESBRECHT², MATTHIAS HANDLOSER², PABLO DOCAMPO², HEINZ KALT¹, and MICHAEL HETTERICH¹ — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — ²Department of Chemistry and Center for NanoScience, University of Munich (LMU), 81377 München, Germany

Organic-inorganic halide perovskites show an outstanding performance as absorber material in solar cells due to their strong absorption coefficient, low non-radiative carrier recombination and simple low-cost production methods. With temperature-dependent absorption measurements and photoluminescence spectroscopy from 10 K to room-temperature we can gain information on structural and optical properties of the material system which is important for a better understanding of the physical processes in the absorber material. In this contribution we study $\text{CH}_3\text{NH}_3\text{Pb}(\text{I}_{1-x}\text{Br}_x)_3$ and investigate the composition-dependent band-gap variation which is useful for band-gap tuning in solar cells. The material system undergoes a phase transition from the low-temperature orthorhombic phase to the tetragonal phase at 150-165 K depending on the halide composition. On the basis of the temperature-dependent absorption and photoluminescence measurements above 170 K, where the tetragonal phase seems to be stable, an upper limit for the exciton binding energy of methyl ammonium lead iodide can be estimated.

HL 90.19 Thu 16:00 Poster A

Electrical Characterization of Methylammonium Tin Iodide Layers as Photovoltaic Absorbers — ●JONAS HORN, MANUEL WEISS, CHRISTOPH RICHTER, and DERCK SCHLETTWEIN — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany.

The preparation of absorber layers composed of methylammonium tin iodide ($\text{CH}_3\text{NH}_3\text{SnI}_3$) in a two-step process was investigated. The material may serve as a less toxic alternative to $\text{CH}_3\text{NH}_3\text{PbI}_3$ as active material in perovskite solar cells. Tin(II) iodide layers prepared by physical vapor deposition on microstructured Au electrode arrays on SiO_2/Si were converted to $\text{CH}_3\text{NH}_3\text{SnI}_3$ by reaction with a spin-coated solution of methylammonium iodide. The perovskite particles were over 200 nm in size and the films reached almost complete surface coverage. The material absorbs over a broad part of the solar spectrum, broader even than $\text{CH}_3\text{NH}_3\text{PbI}_3$. An average resistivity of 26 Ohm cm was measured, characteristic of semiconducting rather than metallic $\text{CH}_3\text{NH}_3\text{SnI}_3$, which speaks in favor of the suitability for photovoltaic applications. The excellent stability of the resistivity, at least within the inert atmosphere of the glove box, and the independently proven stability of the film structure even after contact to air show the good prospects for applications as absorber layers in perovskite solar cells.

HL 90.20 Thu 16:00 Poster A

Characterisation of photoluminescence and absorption in hybrid perovskite thin films — ●SETH NIKLAS SCHUMANN, SEBASTIAN REICHERT, ALEXANDER WAGENFAHL, and CARSTEN DEIBEL — Fakultät für Naturwissenschaften, TU Chemnitz, D-09126 Chemnitz

In the last few years the organic-inorganic hybrid perovskite solar cells

came to attention due to their impressive power conversion efficiency increase to above 20%. They also are expected to have low manufacturing cost. To take advantage of the potential the hybrid perovskites have to offer for photovoltaics we need to characterise the active layer regarding layer homogeneity and optical properties. For our active layers we used the $\text{CH}_3\text{NH}_3\text{PbI}_3$ material system which we processed using the interdiffusion approach. We optimized the processing parameters to obtain homogeneous and pinhole free thin films. We characterised these thin films using photoluminescence, absorption and excitation spectroscopy.

HL 90.21 Thu 16:00 Poster A

Influence of preparation parameters on film morphology and charge transfer in doped organic semiconductors investigated by IR spectroscopy — ●SEBASTIAN BECK^{1,2}, LARS MÜLLER^{2,3}, VIPILAN SIVANESAN^{1,2}, and ANNEMARIE PUCCI^{1,2} — ¹Universität Heidelberg, Kirchhoff-Institut für Physik — ²InnovationLab GmbH, Heidelberg — ³Technische Universität Braunschweig, Institut für Hochfrequenztechnik

Molecular orientation as well as a homogeneous dopant distribution are known to be important for efficient charge transfer (CT) in doped organic semiconductors. Both properties can be varied in a certain range by changing preparation parameters. In this study, the influences of different preparation parameters on film morphology and CT in doped organic semiconductors are investigated. In films deposited onto a cooled substrate in vacuum a reduced diffusion of the evaporated molecules on the substrate surface occurs. The reduced thermal energy of the deposited molecules freezes non-equilibrium molecular orientations of dopant and matrix molecules which prevent efficient CT. During warming up to room temperature a molecular rearrangement takes place facilitating CT in the doped layer. This effect is studied and identified by means of in-situ IR spectroscopy. The morphologies of solution processed thin films are varied by spin coating doped layers from solvents with different polarities and evaporation temperatures. Observed differences in UV-Vis spectra of doped P3HT solutions and thin layers prepared from these solutions indicate a pre-definition of the thin film morphology already in the liquid phase.

HL 90.22 Thu 16:00 Poster A

Improving electron injection and stability of metal electrodes in organic electronic devices with self-assembled monolayers on printing-relevant time-scales — ●SABINA HILLEBRANDT^{1,2}, MILAN ALT^{2,3}, JANUSZ SCHINKE^{2,4}, MALTE JESPER⁵, and ANNEMARIE PUCCI^{1,2} — ¹Heidelberg University, KIP — ²InnovationLab GmbH, Heidelberg — ³Karlsruhe Institute of Technology, LTI — ⁴TU Braunschweig, Inst. f. Hochfrequenztechnik — ⁵Heidelberg University, OCI

In organic semiconductor devices charge injection at the interface is important for the device performance. Charge injection can be improved by controlling the energy alignment at the interfaces, especially between metal contact and organic semiconductor. The thickness of these layers has to be very well defined to avoid any insulating or doping effects. Self-assembled monolayers (SAMs) in this case offer a beneficial way to produce such layers.

In our studies we work with molecules that allow a work function (WF) reduction of about 1.2eV on Gold and Silver contacts. Effects on the WF shift due to molecular orientation are investigated by IR reflection-absorption spectroscopy, the WF is investigated by Kelvin Probe measurements and photoelectron spectroscopy. Devices are fabricated focussing on printing feasibility and the improvement of device life time.

HL 90.23 Thu 16:00 Poster A

Transient localization in rubrene — ●MICHAEL GEIGER¹, ANDREA ROHWER¹, MARTIN DRESSEL¹, UTE ZSCHIESCHANG², HAGEN KLAUK², TERESA SCHMEILER³, and JENS PFLAUM³ — ¹Physikalisches Institut, Universität Stuttgart, Germany — ²Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — ³Experimentelle Physik VI, Universität Würzburg, Germany

Rubrene single crystals consist of van der Waals bound polycyclic aromatic hydrocarbons. Intrinsically, rubrene is an insulator, but can become conductive by e.g. field-effect doping. As such rubrene single crystals have shown highest room-temperature hole mobilities of about 20 cm²/Vs. Due to these properties rubrene has gained attention over the last years and appears to be a promising candidate for electronic applications such as field effect transistors (FETs) in active matrix displays.

We study the fundamental mechanisms that govern charge carrier

transport in rubrene and that are still under debate. In particular, by the thermal motion of molecules the electronic wave function can localize on time scales corresponding to these molecular vibrations and charge transport has to be modelled by transient localization. To verify this theory for organic semiconductors we measure the hole mobility as a function of temperature in FETs composed of ultra pure rubrene crystals as active transport layer and compare the results to calculations [1]. In the next step we investigate these FETs by IR spectroscopy to trace the dynamical behaviour of charges and their excitation by pulsed lasers.

[1] S. Fratini, S. Ciuchi & D. Mayou, Phys. Rev. B 89, 235201 (2014)

HL 90.24 Thu 16:00 Poster A

Accessing charge transfer dynamics in Merocyanine:PCBM blends using NIR-VIS transient absorption spectroscopy — ●KESTUTIS BUDZINAUSKAS¹, LENA WYSOCKI¹, DIRK HERTEL², KLAUS MEERHOLZ², and PAUL H.M. VAN LOOSDRECHT¹ — ¹II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77 50937 Köln — ²Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, 50939 Köln

Merocyanine based dyes are good model materials to investigate charge generation mechanisms in donor:acceptor blend systems. The power conversion efficiency of organic solar cells is a complex parameter, which usually strongly depends on microscopic processes involving for instance interfacial charge transfer states and the formation of long lived triplet states. Fundamental understanding of these effects is critical in order to design new high conversion efficiency solar cells. Here, we study these processes on their intrinsic timescale using time resolved VIS-NIR spectroscopy methods. We focus on the charge formation dynamics in solution processed merocyanine:PCBM blends as well as in merocyanine single crystals and extract quantitative information on the charge transfer dynamics between different excited species.

HL 90.25 Thu 16:00 Poster A

Temperature Dependent Charge-Transfer-State Spectroscopy of Organic Solar Cells — ●CLEMENS GÖHLER and CARSTEN DEIBEL — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

In nowadays often used bulk-heterojunction solar cells, the separation of excitons is aided by adding an acceptor material to the absorbing donor, forming an interfacial state at which charge transfer can take place. This charge-transfer or CT-state can be excited directly with sub-bandgap photons and serves as the main radiative recombination pathway when the solar cell is used as a light emitting diode.

By examining both effects via external quantum efficiency (EQE) and electroluminescence (EL) spectroscopy, one can learn more about the nature of charge-carrier separation and recombination in organic solar cells, which are considered main effects for the losses in the open-circuit voltage (V_{oc}).

To contribute, we examine both the EQE and EL of organic solar cells with varying V_{oc} as a function of the ambient temperature to reduce homogeneous broadening of the CT-absorption and emission lines. Thus, we have an access to the Marcus Theory's molecular reorganization energy and their influence on the V_{oc} -losses.

HL 90.26 Thu 16:00 Poster A

Characterisation of loss mechanisms in hybrid trihalide perovskite solar cells — ●SEBASTIAN REICHERT, SETH NIKLAS SCHUMANN, ALEXANDER WAGENPFAHL, and CARSTEN DEIBEL — Fakultät für Naturwissenschaften, TU Chemnitz, D-09126 Chemnitz

Organic-inorganic trihalide perovskite solar cells belong to the most significant developments in the field of photovoltaics in the last years and seem to be a good bet at satisfying the need for high efficiencies and low manufacturing cost.

To take advantage of the potential of these hybrid solar cells, the loss mechanism which occurs within the active layer need to be understood. We therefore measure current-voltage characteristics for a range of perovskite ($\text{CH}_3\text{NH}_3\text{PbI}_3$) solar cells with different processing parameters. We investigate the photoluminescence transients on corresponding thin films without electrodes. The loss mechanisms are modeled by fitting the obtained data to the continuity equation for excitons and charge carriers. We finally correlate the found recombination losses to the extracted solar cell parameters.

HL 90.27 Thu 16:00 Poster A

The Influence of Morphology and Interface Treatment on

Organic 6,13 bis(triisopropylsilylethynyl)-Pentacene Field-Effect Transistors — ●DANIEL BÜLZ, FRANZISKA LÜTTICH, SREETAMA BANERJEE, GEORGETA SALVAN, and DIETRICH R. T. ZAHN — Semiconductor Physics, Technische Universität Chemnitz, Germany

For the development of electronics, organic semiconductors are of great interest due to their adjustable optical and electrical properties. Aiming for simpler fabrication processes, we investigate TIPS-pentacene organic field effect transistors (OFETs) made from solution with different techniques. Because of the different deposition methods, the TIPS-pentacene thin films exhibit different morphologies in terms of crystal size and homogeneity of the substrate coverage. Additionally, the interface treatment is known to have a strong influence on the threshold voltage, eliminating trap states of silicon oxide at the gate electrode and thereby changing the electrical switching response of the transistors. We therefore investigate the influence of interface treatment using either octadecyltrichlorosilane (OTS) or a simple cleaning procedure with acetone, ethanol, and deionized water. The transistors consist of prestructured OFET substrates including gate, source, and drain electrodes, on top of which TIPS-pentacene dissolved in a mixture of tetralin and toluene is deposited by spray-, or spin-coating. The OFETs are characterized by means of optical microscopy (in order to determine the overall quality of the sample, i.e. crystal size and coverage of the channel region) and electrical transport measurements.

HL 90.28 Thu 16:00 Poster A

Confocal photoluminescence measurements of the charge transfer state in diluted bulk heterojunctions — ●MARTIN STREITER, ALEXANDER WAGENPFAHL, and CARSTEN DEIBEL — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

The understanding of recombination mechanisms at donor-acceptor interfaces is of high importance for improving organic solar cells, as they determine the open circuit voltage and influence the photocurrent. In order to investigate the local properties of charge transfer (CT) states in view of nongeminate losses, we studied diluted bulk heterojunction films.

Photoluminescence spectroscopy was performed using a confocal laser scanning microscopy setup with cryostat sample stage to collect spatially resolved CT emission with sub-micron resolution. Spin coated TAPC-C₆₀ and TAPC-PCBM films with less than 1 mol% acceptor concentration were studied. We investigated the connection between structural information, e.g. acceptor material cluster formation, to CT emission and discuss the results with respect to thermal activation and energetic disorder.

HL 90.29 Thu 16:00 Poster A

Solution Processed TIPS-pentacene/Au Hybrid Trench Devices for Light Sensing Applications — ●SREETAMA BANERJEE^{1,2}, DANIEL BÜLZ¹, DANNY REUTER², KARLA HILLER², DIETRICH R. T. ZAHN¹, and GEORGETA SALVAN¹ — ¹Semiconductor Physics, Technische Universität Chemnitz, Germany — ²Zentrum für Mikrotechnologien, Technische Universität Chemnitz, Germany

Organic-inorganic hybrid electronics can combine the advantages offered by either organic or inorganic materials individually and thereby exhibit enhanced performance. In this work, we present 6,13-bis(triisopropylsilylethynyl)-Pentacene solution-processed planar type organic/inorganic hybrid devices with trench isolated gold electrodes. Devices with organic channel dimensions of 100 nm - 260 nm were fabricated by UV lithography and drop-coating using a TIPS-pentacene solution. The electrical characterization of such devices was carried out with and without illumination to check for possible applications of such devices in light sensing. Three different laser lines (325 nm, 514.7 nm, and 632.8 nm) were used for illuminating the sample. It was observed that the photocurrent and photo-switching response time increases with the photon energy. Devices with smaller channel length showed higher photocurrents and faster switching behaviour. This observation is in agreement with the presence of space charge limited currents as a main transport mechanism.

HL 90.30 Thu 16:00 Poster A

Efficient dissociation of charge transfer states in PTB7-based organic solar cells — ●MARINA GERHARD¹, ANDREAS P. ARNDT², IAN A. HOWARD³, MÜHENAD BILAL¹, ARASH RAHIMI-IMAN¹, ULI LEMMER^{2,3}, and MARTIN KOCH¹ — ¹Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany — ²Light Technology Institute, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — ³Institute of Microstruc-

ture Technology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

In organic solar cells, interfacial charge transfer (CT) states can either act as precursors for free charges or possess trapping character, enhancing geminate recombination. Here, we present a study on the polymer PTB7, blended with the fullerene derivative PC₇₁BM, where we investigate interfacial recombination by means of time-resolved photoluminescence^[1]. Our results on the temperature- and energy-dependent decay dynamics suggest that there is a kinetic competition between charge separation and CT recombination. We find low activation barriers for CT quenching in the range of $k \cdot T$ at room temperature, indicating that the CT states are only weakly bound. This is consistent with our recent experimental work on field-induced CT quenching. Furthermore, we observe that the nanomorphology has a strong influence on the efficiency of charge separation, because the CT emission yield is much higher after selective excitation of the polymer rather than for preferential excitation of pure fullerene domains.

[1] J. Phys. Chem. C, DOI: 10.1021/acs.jpcc.5b09842 (2015)

HL 90.31 Thu 16:00 Poster A

Revealing spin pair processes in organic solar cells — ●ALEXANDER J. KUPIJAI, FLORIAN G. SCHAEBLE, MARTIN STUTZMANN, and MARTIN S. BRANDT — Walter Schottky Institut und Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching

Further improvements of the efficiency of organic solar cells are expected e.g. from advances in chemistry and the optimization of charge carrier transport. We have previously demonstrated that pulsed electrically detected magnetic resonance (pEDMR) and especially electron double resonance (ELDOR) can be used to identify polaron pair recombination as the rate-limiting spin-dependent charge transport mechanism in P3HT/PCBM solar cells at 10 K. We have shown that these multi-frequency measurements can be extended to solar cells containing other polymers such as PCDTBT, where the same polaron pair recombination is observed, suggesting that this recombination is typical for organic solar cells at low temperatures. At room temperature the situation is different, as the negative polaron peak vanishes. Instead, a signal at lower magnetic fields is tentatively attributed to polarons in PEDOT:PSS, which is used as a hole transport layer in the solar cell studied. Again, we use single- and multi-frequency pEDMR techniques to identify the pair processes leading to spin-dependent transport in order to provide information for an optimization of overall solar cell efficiencies.

HL 90.32 Thu 16:00 Poster A

Multilayer fullerene-free organic solar cells with low energy losses — ●VASILEIOS CHRISTOS NIKOLIS, DONATO SPOLTORE, JOHANNES BENDUHN, FELIX HOLZMÜLLER, CHRISTIAN KÖRNER, and KOEN VANDEWAL — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01069 Dresden, Germany

The generation of free charge carriers at interfaces between organic electron donors (D) and electron acceptors (A) can be very efficient, enabling organic solar cells with external quantum efficiencies (EQE) higher than 80 % and internal quantum efficiencies (IQE) approaching 100 %. On the other hand, recombination of free charge carriers at the D-A interface reduces the open-circuit voltage, and overall power conversion efficiency (PCE) of photovoltaic devices comprising such interfaces.

In this study, we introduce an optimization route in order to improve the V_{oc} in multilayer organic solar cells. The deposition of an ultrathin interlayer between D and A creates a discontinuous layer which reduces the D-A interface area and thus free carrier recombination, while keeping a high free carrier generation yield. Investigating a series of interlayers and multilayer device architectures, we achieve PCE's > 7.5 %. Most notably, this strategy enables a V_{oc} of 1.18 V with a peak external quantum efficiency of 78 % at 1.77 eV (700 nm). Such high quantum efficiencies combined with the very low voltage losses below 0.59 V are unprecedented for organic solar cells. Furthermore, this work provides clear pathways for the minimization of photon energy losses by manipulation of the organic photovoltaic device architecture.

HL 90.33 Thu 16:00 Poster A

Ab-initio simulations of vacancy-impurity complexes in carbon allotropes — ●ALEJANDRO MARTINEZ-SORIA GALLO^{1,2}, ANDREAS GRUENEIS¹, HELMUT FEDDER², THOMAS GRUBER¹, and JOERG WRACHTRUP² — ¹Max Planck Institut für Festkörperforschung, Stuttgart, Germany — ²3rd physics institute, University of Stuttgart,

Stuttgart, Germany

Nitrogen Vacancy defects in diamond have become over the last years an important candidate for a bulk room temperature quantum information processing device. In this poster we investigate the feasibility of approximate density functional theory calculations for describing optical and electronic properties for several vacancy-impurity complexes in different carbon allotropes.

HL 90.34 Thu 16:00 Poster A

Quantum technology application with the silicon-vacancy centre in diamond — ●ANDREAS DIETRICH¹, KAY JAHNKE¹, LACHLAN ROGERS¹, JUNICHI ISOYA², FEDOR JELEZKO¹, and ALEXANDER KUBANEK¹ — ¹Institute for Quantum Optics, University Ulm, Germany — ²National Institute for Materials Science, Namiki, Tsukuba, Ibaraki, Japan

Colour centres in diamond appeared as important and valuable quantum systems for emerging quantum technologies, including the fields of quantum processing, quantum key distribution quantum communication, information processing, quantum metrology and many more. Recently a new color centre showed up to be promising in the fields of single photon generation, flying qubit entanglement and quantum repeater, the silicon vacancy center (SiV⁻) in diamond. Latest work on SiV⁻ has shown its exceptional and promising spectral properties. These qualities leads to efforts to apply these system in quantum technologies. Nevertheless for these purposes some features and effects are still not fully understand. We show how our progress leads to a deeper understanding and to more sophisticated applications of the silicon vacancy centre in diamond.

HL 90.35 Thu 16:00 Poster A

FPGA based measurements of optical properties of silicon-vacancy (SiV) centers in diamond — ●SIMON RUPP¹, ANDREAS DIETRICH¹, ANDREA KURZ¹, KAY JAHNKE², LACHLAN ROGERS¹, JUNICHI ISOYA¹, FEDOR JELEZKO¹, and ALEXANDER KUBANEK¹ — ¹Institute for Quantum Optics, University Ulm, Germany — ²National Institute for Materials Science, Namiki, Tsukuba, Ibaraki, Japan

In the last decades, colour centres in diamond has shown perfect optical properties for quantum information processes. Especially, the silicon-vacancy (SiV) centers with high brightness, narrow bandwidth and spectral stability can be used as an excellent source of indistinguishable single photons. To observe and control the optical properties of such colour centres in real time, a suitable system is required. The FPGA (Field Programmable Gate Array) technology has the ability to implement physical parallel and independent processes in real time. Furthermore, independent tasks can be processed simultaneously on a FPGA which can't be achieved with commercial devices. This gives us the possibility to measure and control the optical properties of silicon-vacancy (SiV) centers in diamond with FPGA technology.

HL 90.36 Thu 16:00 Poster A

Mechanical tuning of nuclear spins in Si — ●MORITZ P.D. PFLÜGER, DAVID P. FRANKE, and MARTIN S. BRANDT — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

Nuclear spins of ionized donors in silicon have many properties that make them interesting for quantum computing applications, especially as a quantum memory. They are compatible with silicon technology, scalable, and possess very long coherence times [1]. However, due to their good isolation, it is difficult to address them selectively. This becomes possible for heavier donors, such as ⁷⁵As, via their quadrupole moment which interacts with electric field gradients which in turn can be tuned by applying elastic strain to the host crystal [2].

We measure pulsed electrically detected electron nuclear double resonance of arsenic-doped silicon, a technique allowing to observe nuclear magnetic resonance phenomena via monitoring the change in conductivity. We extend earlier experiments by applying stress to the samples via piezoelectric actuators, discuss the resonance shifts achievable, and explore the influence of strain on the decoherence of the ⁷⁵As⁺ nuclear spins.

[1] M. Steger, K. Saedi, M. L. W. Thewalt, J. J. L. Morton, H. Riemann, N. V. Abrosimov, P. Becker, and H.-J. Pohl, *Science* **336**, 1280 (2012).

[2] D. P. Franke, F. M. Hrubesch, M. Künzler, H.-W. Becker, K. M. Itoh, M. Stutzmann, F. Hoehne, L. Dreher, and M. S. Brandt, *Phys. Rev. Lett.* **115**, 057601 (2015).

HL 90.37 Thu 16:00 Poster A

Influence of ²⁹Si nuclear spins on the coherence of ionized phosphorus donors in silicon — ●ANDREAS M. RAUSCHER, DAVID P. FRANKE, and MARTIN S. BRANDT — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

The fragility of quantum mechanical states is one of the main obstacles for the physical implementation of quantum bits (qubits). Promising candidates for the latter are the spins of impurities in silicon. In this case, the interaction with ²⁹Si nuclear spins generally acts as the main source of decoherence. Removing this isotope in isotopically controlled ²⁸Si, a record-breaking coherence time of 39 minutes for ³¹P⁺ nuclear spins has been achieved^[1]. Using pulsed electrically detected magnetic resonance (pEDMR) and electron nuclear double resonance (ENDOR), we are able to access the nuclear spin states of both ³¹P⁺ and ²⁹Si in γ -irradiated silicon with natural isotope composition, based on spin pairs formed between donors and irradiation defects (SL1)^[2]. Here, we apply hyperpolarization techniques demonstrated on ³¹P⁺^[3] to ²⁹Si coupled to SL1 and the possibility to use this approach to systematically study the effects of ²⁹Si spins on the decoherence of ³¹P⁺ nuclei.

[1] Kamyar Saedi et al., *Science* **342**, 830 (2013)

[2] David P. Franke et al., *Phys. Rev. B* **89**, 195207 (2014)

[3] Felix Hoehne et al., *Phys. Rev. Lett.* **114**, 117602 (2015)

HL 90.38 Thu 16:00 Poster A

Optical spectroscopy of vacancy related defects in silicon carbide generated by proton irradiation — ●C. KASPER¹, H. KRAUS^{2,1}, A. SPERLICH¹, D. SIMIN¹, T. MAKINO², S.-I. SATO², T. OHSHIMA², G. V. ASTAKHOV¹, and V. DYAKONOV^{1,3} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Japan Atomic Energy Agency, Takasaki, Gunma, Japan — ³ZAE Bayern, 97074 Würzburg

Defects in silicon carbide (SiC) received growing attention in recent years^[1,2,3,4], because they are promising candidates for spin based quantum information processing. In this study we examine silicon vacancies in 4H-SiC crystals generated by proton irradiation. By the use of confocal microscopy the implantation depth of Si vacancies for varying proton energies can be verified.

An important issue is to ascertain the nature and distribution of the defects. For this purpose, we use the characteristic photoluminescence spectrum of Si vacancies, whose intensity is proportional to the defect density. Using xyz-scans, where the photoluminescence at each mapping point is recorded, one can thus determine the vacancies nature and their distribution in the SiC crystal. Additionally we verify the nature of the examined defects by measuring their uniquely defined zero-field-splitting by using ODMR associated with defect spins.

[1] H. Kraus et al., *Nature Phys.* **10**, 157 (2014)

[2] D. J. Chrystle et al., *Nature Mater.* **14**, 160 (2015)

[3] M. Widmann et al., *Nature Mater.* **14**, 164 (2015)

[4] A. Lohrmann et al., *Nature Comm.* **6**, 7783 (2014)

HL 90.39 Thu 16:00 Poster A

Generation of Nitrogen Vacancy Centers in Diamond by Focused Ion Implantation — ●JOHANNES LANG, BORIS NAYDENOV, and FEDOR JELEZKO — Institut für Quantenoptik, Universität Ulm, Germany

The color center in diamond formed by a substitutional nitrogen and an adjacent vacancy (NV center) is amongst the most studied defects in diamond and a promising candidate for different applications such as e.g. qubit spin registers in future quantum computers [1], or as magnetic and electric field sensors [2]. The targeted creation of these NVs is essential for the described applications [3]. We present a UHV-setup for low energy focused ion implantation of nitrogen in order to create NV centers. By adjusting the implantation energy and fluence, the generation depth of up to 20 nm below the surface of the diamond substrate, as well as the NV density and position can be controlled.

[1] J. Scheuer et al., *New J. Phys.* **16** 093022 (2014) [2] C. Müller et al., *Nat. Comm.*, **5** 4703 (2014) [3] J. Meijer et al., *Appl. Phys. Lett.* **87**, 261909 (2005)

HL 90.40 Thu 16:00 Poster A

Mechanical and vibrational properties of strained carbon nano-materials — ●ALEXANDER CROY¹, CHRISTIAN WAGNER², and JÖRG SCHUSTER³ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²Center for Microtechnologies, TU Chemnitz, Germany — ³Fraunhofer Institute ENAS, Chemnitz, Germany

The introduction of carbon nanomaterials, like carbon nanotubes and graphene, into modern nano-electronic architectures is a wide field of application-oriented research — and requires reliable, non-destructive and fast characterization techniques to quantify defects and (local) strain. Optical spectroscopy, such as Raman spectroscopy, to indirectly probe phonons (vibrations), play a major role in this field.

Thus, a detailed understanding of the influence of defects and strain on Raman spectra is required, but the full *ab-initio* description of the coupled optical and phonon interaction is usually not feasible. Therefore, the problem is restricted to the main contribution by phonons — which are typically calculated by means of molecular dynamics (MD).

To maintain *ab-initio* accuracy, we compare the elastic properties of ideal and defective carbon nanostructures obtained by density functional calculations and different carbon force-fields. Within (static) numerical stretching experiments, we focus in particular on nonlinear contributions in the stress-strain-relation. Using MD calculations we study the strain- and defect dependence of the dominant phonon modes, i.e., their frequencies and life-times. Finally, we discuss consequences for Raman spectra.

HL 90.41 Thu 16:00 Poster A

Characterization of diamondoids by Raman spectroscopy — •DOMINIQUE B. SCHUEFFER¹, ANDREY A. FOKIN², PETER R. SCHREINER², and PETER J. KLAR¹ — ¹Institute of Experimental Physics I, Justus Liebig University Giessen, Germany — ²Institute of Organic Chemistry, Justus Liebig University Giessen, Germany

Diamondoids, like adamantane, are the smallest building blocks of diamonds and are currently used to form new molecules by linking these sp³-bonded units to larger cages. Raman spectroscopy is used to characterize various diamondoids as well as the newly formed materials. In particular, in wavelength and polarization dependent Raman experiments the number of modes and their corresponding signal intensity vary, allowing to study the symmetry characteristics and scattering probabilities of the Raman active modes. The vibrational structure of

diamondoids and the more complicated coupled diamondoid molecules give insight into the molecule symmetry and electronic structure. Beside this fundamental point of view diamondoids are of great interest as propellant for radiofrequency ion thrusters, because they are available in abundance and match the required properties. Raman spectroscopy could be used to characterize the residual components of the thruster propellant.

HL 90.42 Thu 16:00 Poster A

Investigations into Optoelectronic Properties of Carbon Nitrides for Solar Hydrogen Production — •FILIP PODJASKI¹, JUAN GALISTEO-LÓPEZ², BRIAN TUFFY¹, KATHARINA SCHWINGHAMMER¹, HERNÁN MÍGUEZ², and BETTINA V. LOTSCH^{1,3} — ¹Max-Planck-Institute for Solid State Research, Stuttgart, Germany — ²Institute of Material Science of Sevilla, Sevilla, Spain — ³Department of Chemistry, University of Munich (LMU), Munich, Germany

Since the discovery of water splitting on TiO₂ under UV-illumination by Honda and Fujishima in 1970s, a lot of materials and cocatalysts have been investigated to produce hydrogen from water using sunlight. A recent discovery has shown that carbon nitrides, consisting only of abundant elements, are able to perform visible light-driven hydrogen evolution. Our research focuses on the understanding and enhancement of charge transfer properties in these semiconducting polymers that lead to improved hydrogen evolution. Time resolved photoluminescence measurements suggest the use of a more general approach than used nowadays in literature to describe the complex decay processes after photo-excitation. Our results reveal how the particle size, the presence of sacrificial donors and how cocatalysts attached to the surface influence the lifetimes of excited states. This findings may lead to a better understanding of the different environmental contributions in homogeneous catalysis and can be used to achieve better charge transfer properties using these materials in heterojunctions for visible light water splitting.