HL 12: HL Poster I

Time: Monday 17:30–20:00 Location: Poster E

HL 12.1 Mon 17:30 Poster E

Charge transport in bottom-up synthesized graphene nanoribbon networks — Alexander Tries[1,2,3], •Leo Schnitzspan[1], Nils Richter[1], Zongping Chen[2], Kamal Asadi[3], Akimitsu Narita[3], Klaus Müllen[3,4], and Mathias Kläui[1,2] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz — [2]Graduate School of Excellence Materials Science in Mainz — [3]Max Planck Institute for Polymer Research — [4]Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz

Graphene nanoribbons (GNRs) attract attention due to particular physical properties resulting from the geometrical confinement, and these also depend crucially on both width and edge morphology [1]. Using GNR field-effect transistors, we perform a systematic study on the electronic properties of chemically synthesized and atomically perfect armchair GNRs with a width of 5 and 9 carbon atoms (5-AGNR and 9-AGNR)[2]. Our measurements reveal nuclear tunneling-assisted charge carrier hopping [3] as the dominant charge transport mechanism allowing us to apply a universal scaling law valid for charge transport in networks of both GNR structures over a large range of driving voltages and temperatures. Gate-dependent measurements show a pronounced hysteretic effect and we identify the origin of this hysteresis by temperature dependent measurements[4,5].

[1] Son et al., Phys.Rev.Lett.97, 216803 (2006). [2] Z. Chen et al., J.Am.Chem.Soc., 139, 9483-9486 (2017). [3] K. Asadi et al., Nat.Commun. 4:1710 (2013). [4] N. Richter et al., arXiv:1806.00962 [5] A.Tries et al., submitted (2018)

HL 12.2 Mon 17:30 Poster E

Defect-induced photoluminescence of WS_2 monolayers — •Aswin Asaithambi[1], Roland Kozubek[1], Guenther Prinz[1], Francesso Reale[2], Cecelia Mattevi[2], Marika Schleberger[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [2]Department of Materials, Imperial College London, London, UK

The transition metal dichalcogenide tungsten di-sulphide (WS_2) has a layered structure with an indirect band gap, which becomes direct at the K point in momentum space if only a monolayer is present. This leads to strongly enhanced photoluminescence (PL), compared to the bulk. However, WS_2 monolayers are not defect free and the defects present in the material affect their emission properties drastically, which makes it necessary to study and characterize their influence.

In this contribution, we present highly sensitive, non-destructive, temperature- and power- dependent PL measurements to study defects in WS_2 monolayers. WS_2 monolayers were irradiated with different fluences of Xe^{30+} ions to create defects (presumably S and W vacancies) with different densities. Room temperature (RT) PL shows no defect-bound emission. Low temperature (LT) PL spectra of irradiated samples show new defect-related emission lines. Interestingly, those new defect-related peaks were annealed when subjected to higher laser power at both RT and LT. These results will be discussed in the frame of excitons, vacancy defect states and possible adsorbates, and compared with literature.

HL 12.3 Mon 17:30 Poster E

Probing long-lived spin polarization in n-doped $MoSe_2$ monolayers. — •Michael Kempf[1], Markus Schwemmer[1], Philipp Nagler[1], Andreas Hanninger[1], Christian Schüller[1], and Tobias Korn[2] — [1]University Regensburg, 93053 Regensburg Germany — [2]University Rostock, 18051 Rostock Germany

With the coupling of spin and valley degree of freedom in transition metal dichalcogenides, these materials are very well suited for valleytronics. Yet due to ultrafast exciton recombination times on the order of picoseconds, strongly limiting possible applications and other processes, it is highly advantageous to transfer the polarization to resident carriers. Utilizing time-resolved Kerr rotation we study the spin-valley dynamics in undoped and n-doped $MoSe_2$ monolayers. In contrast to undoped samples we observe a long-lived polarization of several nanoseconds in the n-doped $MoSe_2$, which can be explained by a polarization of resident carriers. M. Schwemmer et al., Appl. Phys. Lett. **111** (2017)

HL 12.4 Mon 17:30 Poster E

Edge currents driven by terahertz radiation in graphene in the quantum Hall regime — •Susanne Candussio[1], Helene Plank[1], Mikhail Durnev[2], Johanna Pernul[1], Kathrin-Maria Dantscher[1], Erwin Mönch[1], Andreas Sandner[1], Jonathan Eroms[1], Dieter Weiss[1], Vasily V. Belkov[2], Sergey A. Tarasenko[2], and Sergey Ganichev[1] — [1]Terahertz Center, University of Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia

We observe that the illumination of unbiased graphene in the quantum Hall regime with polarized terahertz laser radiation results in a direct edge current. This photocurrent is caused by an imbalance of persistent edge currents, which are driven out of thermal equilibrium by indirect transitions within the chiral edge channel. The direction of the edge photocurrent is determined by the polarity of the external magnetic field, while its magnitude depends on the radiation polarization. The microscopic theory developed in this paper describes well the experimental data.

HL 12.5 Mon 17:30 Poster E

Optical Contrast Analysis and Electrical Properties of Thin $ZrSe_3$-Films — •Lars Thole[1], Christopher Belke[1], Sonja Locmelis[2], Johannes C. Rode[1], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

In recent years interest in two-dimensional materials has been strong. They have a layered structure with unique properties. One type of layered materials are Transition Metal Trichalcogenides of the form MX_3, where M is a transition metal and X is a chalcogenide [1, 2]. We concentrate on the semiconductor $ZrSe_3$ [2, 3]. It was exfoliated to get thin flakes with only a few layers. The flakes were characterized with atomic force microscopy and optical microscopy to determine a contrast relation for the height. Through electrical measurements on contacted flakes the mean free path for the material was determined. Further measurements to determine the mobilities of the flakes were conducted.

[1] J. O. Island et al., 2D Materials, 4, 0220033 (2017).
[2] J. Dai et al., WIREs Comput. Mol. Sci., 6, 211-222 (2016).
[3] Y. Jin et al., Phys. Chem. Chem. Phys., 17, 18665 (2015).

HL 12.6 Mon 17:30 Poster E

Magnetotransport properties of weakly coupled double trilayer graphene — •Xiao Xiao, Sung Ju Hong, Christopher Belke, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany

We have investigated magnetotransport properties of double trilayer graphene (DTLG). The DTLG was fabricated by stacking two trilayer graphene (TLG) flakes. Analyzing the edges of the two flakes in the optical microscope, we identified a large twist angle around 24°. This is consistent with the electrical measurements which show the superposition of two independent magnetotransport properties. As in twisted bilayer graphene, the large twist angle seems to result in a weak coupling between the two layers. In the observed Landau fan diagram, one of the DTLG turns out to be ABA-stacked TLG with broken symmetry states. Furthermore, we found an additional high carrier density which comes from the other TLG.

HL 12.7 Mon 17:30 Poster E

Fabrication of twisted graphene heterostructures: Different layer sequences and novel device configurations — •Benjamin Gajeufsky, Xiao Xiao, Sung Ju Hong, Christopher Belke, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany

Twisted bilayer graphene (tBLG) is a representative van der Waals heterostructure, which shows various electronic properties depending on the twist angle. To date, the heterostructures have been constructed using monolayer graphene. Therefore, heterostructures which consist of different ingredients such as bilayer or trilayer graphene remain elusive. Furthermore, since the observable quantities are also limited to conventional transport properties, distinct measurement configurations may reveal novel kind of electronic properties. Here we expand

the twisted graphene heterostructure in terms of different layer sequences or device configurations.

HL 12.8 Mon 17:30 Poster E

From multi- to monolayer: monitoring the time-evolution of laser-induced thinning of MoS_2 layers by Raman and photoluminescence spectroscopy — •Christian Tessarek, Oleg Gridenco, Jan Müssener, Stephan Figge, Kathrin Sebald, Jürgen Gutowski, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany

Exfoliation of MoS_2 crystals is a simple method to obtain multi- and monolayer material. However, size and number of monolayers produced by this technique are usually small and not well controllable. Laser-thinning is an established method to produce MoS_2 monolayers from multilayers [1]. For a better control of a homogeneous monolayer generation, monitoring of the thinning process is required.

Multi- and monolayers show different distinct properties in Raman and photoluminescence spectroscopy and thus these spectroscopic techniques are suitable to monitor the transition from multi- to monolayer. A laser emitting at 325 or 406 nm is used simultaneously for both thinning and spectroscopy. The time-evolution of the Raman and photoluminescence peaks will show a layer-by-layer etching of MoS_2 and a transformation into amorphous MoO_x in an oxygen containing atmosphere during the thinning process. Microstructuring of multilayers into monolayers such as writing of single points, lines and areas will be demonstrated.

[1] A. Castellanos-Gomez et al., Nano Lett. **12**, 3187 (2012).

HL 12.9 Mon 17:30 Poster E

Strain induced optical effects of WS_2 monolayers — •Marcel Ney, Aswin Asaithambi, Lukas Madauss, Günther Prinz, Marika Schleberger, and Axel Lorke — Faculty of Physics and CENIDE, University Duisburg-Essen, Germany

Two-dimensional transition metal dichalcogenide (TMD) monolayers interact efficiently with visible light due to the direct bandgap nature at K-point in momentum space. The result of the quantum confinement effects in two dimensions is a strong electron-hole Coulomb interaction, leading to a large exciton binding energy, which makes this material very promising for optoelectronic device fabrication.

We will present photoluminescence- (PL) and Raman spectroscopy results of WS_2 monolayers grown on a standard Si/SiO_2 substrate via a chemical vapor deposition (CVD) process.

In PL investigations, we observed a redshift of the excitonic wavelength between the center and the edge of a triangular WS_2 monolayer. These redshifting recombination energies could indicate strain within the monolayer. Therefore complementary Raman spectroscopy measurements were performed, which results support the assumption of a strain induced excitonic redshift. The maximum relative tensile strain was calculated to 1.2%, applying a relation between strain and Raman shift [1].

The influence of strain on the optical properties of WS_2 monolayers at temperatures ranging from 295K to 77K and for different excitation powers will be discussed and compared with results from literature.

[1] F. Wang et al., 2D Mater. 4, 015007 (2016)

HL 12.10 Mon 17:30 Poster E

Induced defect states in supported and freestanding MoS_2 monolayers — •Sven Mehrkens, Oleg Gridenco, Kathrin Sebald, Christian Tessarek, Martin Eickhoff, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Alle 1, D-28359 Bremen, Germany

Single-layer molybdenum disulfide (MoS_2) photoluminescence emission is strongly affected by the dielectric environment, i.e., of the supporting substrate. To avoid this, it is highly preferable to study the optical properties of freestanding monolayers. In this contribution an etching-free transfer method using polymethyl-methacrylate (PMMA) will be demonstrated, for the transfer of mechanically exfoliated MoS_2 flakes from SiO_2 substrates to a TEM grid. Localized excitons, trapped at vacancies are of considerable importance for the characteristics of optoelectronic devices. In MoS_2, vacancies can be introduced via Ga^+ ion irradiation using a focused ion beam (FIB). A variation of the ion dose results in different densities of defect states, emitting at 1.75 eV for flakes on SiO_2 at 4 K. We compare the optical properties of freestanding and supported monolayers in order to investigate the influence of the dielectric environment on the introduced defect states.

HL 12.11 Mon 17:30 Poster E

Raman spectra vs. transport properties in graphene field-effect transistors suitable for applications in ultrasensitive biodetection — •Daniel Hüger[1], David Kaiser[1], Christof Neumann[1], Thomas Weimann[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich-Schiller-University Jena, 07743 Jena, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

For applications of graphene field-effect transistors (GFETs) in ultrasensitive biodetection the devices must have a high charge carrier mobility, a low doping level as well as an absence of the transfer curves hysteresis. To study these properties, extensive and time-consuming transport measurements in vacuum are typically required. Here, in order to find a faster and non-invasive method for this assessment, we use Raman spectroscopy to characterize GFETs fabricated on Si/SiO_2 wafers and correlate the spectroscopy and transport data. We present an analysis of over 600 FET devices made by electron-beam lithography from single-layer graphene produced via chemical vapor deposition (CVD) by three different manufacturers. Employing a spectral resolution of $\sim$10 cm^{-1}, we acquire the Raman data within only 3 minutes per sample. We analyze the relationships between hysteresis in the transfer curves, position of the Dirac-point and charge carrier mobility in the GFETs with position of the 2D-, D- and G-peak, their full width half maximum (FWHM) and intensity ratios.

HL 12.12 Mon 17:30 Poster E

Enhanced Photoluminescence from Monolayer WS2 Excitons with a 2D-material-air-GaP in-plane Microcavity — Oliver Mey[1], Franziska Wall[1], •Lorenz Maximilian Schneider[1], Frederik Walla[2], Amin Soltani[2], Hartmut G. Roskos[2], Ni Yao[3], Peng Quing[3], Wei Fang[3], and Arash Rahimi-Iman[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt am Main, Germany — [3]State Key Laboratory of Modern Optical Instrumentation, College of Optical Science and Engineering, Zhejiang University, Hangzhou 310027, China

To improve light-matter interaction with two-dimensional semiconductors for future applications involving monolayer materials in waveguide-coupled on-chip integrated circuitry and valleytronic nanophotonics, we study the effects of tailoring the landscape on which the monolayers are placed. In this context, photoluminescence enhancement from monolayer WS2 on GaP substrates patterned by focused-ion-beam etching was investigated. Here, we present a unique optical microcavity approach, which results in a WS2 photoluminescence enhancement by a factor of 10 at room temperature compared to the unstructured substrate. Here, we combine a bulls-eye-shaped circular Bragg grating, for interference effects in the horizontal direction, and an optimized etching depth of circular air-GaP structures, for maximum constructive interference effects of the applied pump and expected emission light in the vertical direction.

HL 12.13 Mon 17:30 Poster E

Band Gap Determination and Induced Conductivity in Thin Films of ZrS_3 — •Christopher Belke[1], Sonja Locmelis[2], Johannes C. Rode[1], Hennrik Schmidt[1], Bastian Hoppe[2], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

New varieties of two-dimensional crystals [1] are currently getting into focus of the material sciences. An example for such layered materials are Transition Metal Trichalcogenides. Here we study the compound ZrS_3: Bulk crystals were synthesized by chemical gas transport; stoichiometry and structure were verified by powder X-ray diffractometry and energy-dispersive X-ray spectroscopy (EDX) and it was analyzed by absorption measurements. The latter indicate an indirect bandgap of about 1.8 eV and a direct bandgap of 2.3 eV, which differ slightly from literature values [2, 3]. Thin flakes are exfoliated and contacted. Conductivity measurements are investigated in response to illumination with LEDs of different wavelengths. We observe a pronounced rise in conductivity between 2.1 eV and 2.4 eV which is in good agreement with the direct bandgap found in the absorptions measurements. Also with field effect measurements charge carriers could be induced in thin flakes.

[1] A. K. Geim, I. V. Grigorieva, Nature 499, 419-425 (2013).
[2] M. Abdulsalam, D. Joubert, Eur. Phys. J. B. 88, 177 (2015).
[3] Y. Jin, X. Li, J. Yang, Phys. Chem. Chem. Phys. 17, 18665

(2015).

HL 12.14 Mon 17:30 Poster E

Structural Dynamics of Rhenium Disulphide Studied by Ultrafast Electron Diffraction — Arne Ungeheuer, •Ahmed Hassanien, Marlene Adrian, Arne Senftleben, and Thomas Baumert — Institute of Physics and CINSaT, University of Kassel, Heinrich-Plett-Strasse 40, D-34132 Kassel, Germany

Unlike most two-dimensional transition metal dichalcogenides (MoS_2, WSe_2, etc...), rhenium disulphide (ReS_2) shows minor dependence of its electronic and vibrational properties on the number of stacked atomic layers [1]. Its distorted triclinic crystal structure due to in-plane dimerization of Re atoms results in a weak binding energy between its layers and consequently weak coupling. On the other hand, due to this so-called Peierls distortion, ReS_2 shows significant polarization-dependent optical properties which hold promise for such applications as valleytronics [2].

Ultrafast electron diffraction is a continuously developing technique for providing direct insights into photo-induced primary dynamics at the atomic level in molecules and solids. Using a highly compact femtosecond electron diffractometer developed in our group [3], we show our first measurements of the structural dynamics of mechanically-exfoliated few-layer ReS_2 revealed on a picosecond timescale, following the photoexcitation with a femtosecond laser pulse.

References:
[1] Tongay, Sefaattin, et al. Nature communications 5 (2014): 3252.
[2] Cui, Yudong, et al. Scientific Reports 7 (2017): 40080.
[3] Gerbig, C., et al. New J. Phys. 17.4 (2015):043050.

HL 12.15 Mon 17:30 Poster E

Charge transport in graphene and graphene nanoribbons on hexagonal boron nitride as field effect transistor devices — •Leo Schnitzspan[1], Alexander Tries[1,2,3], Marie-Luise Braatz[1], and Mathias Kläui[1,2] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz — [2]Graduate School of Excellence Materials Science in Mainz — [3]Max Planck Institute for Polymer Research

Graphene nanoribbons (GNRs) have attracted attention due to particular physical properties resulting from the geometrical confinement, and these also depend crucially on both width and edge morphology [1]. Hexagonal boron nitride (hBN) has turned out as ideal substrate for graphene due to its flat and similarly lattice structure, which results in charge mobilities up to 275 000 $cm^2V^{-1}s^{-1}$ [2]. Using a field-effect transistor layout with a hBN underlayer, we study the electronic properties of graphene and GNRs and analyze the underlying mechanisms. Different wet and dry graphene transfer methods are tested and developed. Magnetotransport as well as gate-dependent measurements are investigated to understand the impact of hBN on the transport properties.

[1] Son et al., Phys. Rev. Lett. 97, 216803 (2006). [2] Zomer, P. J., et al., App. Phys. Lett. Bd. 99.23 (2011)

HL 12.16 Mon 17:30 Poster E

Metal gate vs graphene gate in two-dimensional (2D) MoS2 FET — •Vaishnavi Kateel[1,2], Zahra Fekri[1,2], Phanish Chava[1,2], Himani Arora[1,2], Kenji Wanatnabe[3], Takashi Taniguchi[3], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden Rossendorf,Bautzner Landstraße 400, 01328 Dresden — [2]Technische Universität Dresden, 01062 Dresden Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

The extensive scaling of semiconducting devices caused the search for alternative materials as the conventional semiconductor reached the edge of their physical limits. Huge research in 2D material was driven by their wide range of electrical properties from metallic to insulating. The interlayer van der Waals interaction allowed 2D materials to be exfoliated and stacked in order to form heterostructure with little lattice mismatch. Layer dependent electronic band structure and the absence of surface dangling bond made semiconducting MoS2 as a good channel material in our 2d transistor. Graphene(Gr) source/drain contacts were used as transport across the schottky barrier of Gr/MoS2 interface can be altered by gate voltage and current bias. Excellent properties like wide bandgap, atomic flatness and absence of charge traps makes hexagonal Boron Nitride (hBN) a better dielectric layer for our 2D FET compared to SiO2 which shows large hysteresis and low mobility. Furthermore, hBN can be used as protection by encapsulating 2D semiconductors. We demonstrate a 2D heterostructure MoS2 transistor with graphene gate electrode and compare its electrical characteristics with metal top-gate electrode MoS2 transistor.

HL 12.17 Mon 17:30 Poster E

Three-dimensional electronic band dispersion in bulk black phosphorus — •Charlotte Sanders[1], Klara Volckaert[2], Deepnarayan Biswas[2], Marco Bianchi[2], Jill Miwa[2], Søren Ulstrup[2], and Philip Hofmann[2] — [1]Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell Campus, Didcot, U.K. — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Aarhus, Denmark

Bulk black phosphorus has a layered structure similar to that of pseudo-two-dimensional materials like graphite and bulk MoS2. However, to a greater extent than in some other layered materials, interlayer interaction plays an important role in determining the electronic properties of black phosphorus, leading to a distinctive kz-dispersing band and a direct band gap of 0.3 eV at the Z point of the Brillouin zone. Investigations by angle-resolved photoemission spectroscopy (ARPES) of the three-dimensional dispersion of nominally undoped black phosphorus have been reported (e.g., [1,2]), but several questions remain unanswered. For example, a surface resonance state has been reported [2]; but whether such a state in fact exists, and what its origin might be, remain in doubt. Furthermore, ARPES measurements have yielded results that differ rather widely from predictions from theory. Here I will present ARPES measurements–spanning the photon energy range hv=15-135 eV–of the three-dimensional band structure of bulk black phosphorus, and I will suggest how our results can address some of the questions which have remained unresolved in the literature so far. [1] PRB 33 (1986) 4324. [2] PRB 90 (2014) 085101.

HL 12.18 Mon 17:30 Poster E

Manipulating transition-metal dichalcogenide monolayers with proximity effects — •Lanqing Zhou, Sven Borghardt, and Beata Kardynal — Forschungszentrum Jülich PGI-9,Jülich, Germany

Transition-Metal Dichalcogenides (TMDs) monolayers have been shown to exhibit many interesting physical properties related to their crystal structure and strong spin-orbit interactions. In addition, being only three atomic planes thin, their properties can be manipulated using proximity fields generated when they are placed in contact with functional molecules or films. Here we interface tungsten diselenide monolayers with thin films of chromium trichlotride and chromium tribromide. Both chromium trihalides are layered materials which are electronic insulators that are also ferromagnetic at low temperatures. As such, they can be used as functional substrates for the monolayer WSe2 to introduce energy splitting of the spin states in K and K* valleys of the monolayer. In this contribution, we study different sample preparation methods to maximize the stability of the chromium trihalide films. We use hexagonal boron nitride to protect the ferromagnetic films from the ambient humidity and thin graphite films to protect the TMD monolayers from the effects of charge fluctuations in the substrate that can cause inhomogeous broadening of the photoluminescence spectra. Effects of the ferromagnetic layers on the monolayers in the devices are investigated using optical spectroscopy at different temperatures.

HL 12.19 Mon 17:30 Poster E

Highly sensitive micro-cavity based absorption spectroscopy of low dimensional materials — •Thomas Hümmer[1,2], Jonathan Noé[3], Alexander Högele[3], Theodor W. Hänsch[1,2], and David Hunger[4] — [1]Ludwig-Maximilians-Universität München, Deutschland — [2]Max-Planck Institut für Quantenoptik, Garching, Deutschland — [3]Fakultät für Physik and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, D-80539 München — [4]Karlsruher Institut für Technologie, Karlsruhe, Deutschland

We use a tunable high-finesse optical micro-cavity [1] to measure absorption in carbon nanotubes (CNTs) and transition metal dichalcogenides (TMDs) down to the parts-per-million level. Our scanning-cavity imaging technique[2,3], where a microscopic mirror is scanned across a larger mirror that hosts the sample, allows to collect absorption images of individual nano-structures with unprecedented sensitivity, spatially resolved with 1*m resolution and in real time. First spectroscopic measurements are performed on these samples. We present our progress to extend this technology to measurements in cryogenic environments. [1] Hunger et al., NJP 12, 065038 (2010) [2] Mader et al., Nat Commun 6, 7249 (2015) [3] Hümmer et al Nat Commun 7, 12155 (2016)

HL 12.20 Mon 17:30 Poster E

First principles study of Ta_2NiSe_5, a possible candidate exci-

tonic insulator, using GW and hybrid functional approaches — •Lukas Windgätter, Simone Latini, Hannes Hübener, and Angel Rubio — Max Planck Institut für die Struktur und Dynamik von Materie

The idea of the excitonic insulator scenario, which describes the electron-hole condensation in thermal equilibrium, was originally proposed by X. Jerome et al. in 1967. It is expected to occur in semiconducting materials with a very small bandgap of a few milli electron volt. Recently it has attracted renewed interest with the discovery of several materials with experimental signature of equilibrium exciton condensation. In this context we are investigating Ta_2NiSe_5, which has shown to be a promising candidate in recent publications, using ab-initio methods. We present results using DFT hybrid functionals as well as ab-initio GW calculations.

HL 12.21 Mon 17:30 Poster E

Optical characterization of implanted transition metal dichalcogenides monolayers — •Minh Bui[1], Jhih-Sian Tu[1], Manuel Auge[2], Sven Borghardt[1], Eoghan O'Connell[3], Ursel Bangert[3], Hans Hofsäss[2], and Beata Kardynał[1] — [1]Peter Grünberg Institut 9, Forschungszentrum Jülich, Jülich, Germany — [2]II. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany — [3]Department of Physics, School of Sciences and Bernal Institute, University of Limerick, Limerick, Ireland

Two dimensional semiconductors, such as monolayers (MLs) of transition metal dichalcogenides, possess some unique properties due to their band structure and geometry. In analogy to classic bulk semiconductors, it is desirable to introduce stable dopant atoms into their lattice in a controlled way for exploiting these properties. In this contribution, we investigate low energy ion implantation as a method to introduce foreign atoms into MoS_2 and $MoSe_2$ MLs. Raman, reflectance and photoluminescence spectroscopies, supported by transmission electron microscopy, are used to characterize the resulting semiconductors. Implantation of Se ions with energies below 50 eV into exfoliated MoS_2 MLs is studied as a prototypical system. Substitution of S with Se atoms should convert MoS_2 into $MoSe_{2x}S_{2(1-x)}$ without generating free charge carriers. Implantation levels of up to few percent, much larger than needed for doping, are shown. We find that implanted ion energy is a compromise between implantation success rate and defect formation rate, and we identify the most likely defects. Similarly, results of $MoSe_2$ implanted with P as an n-type dopant are discussed.

HL 12.22 Mon 17:30 Poster E

Investigation of mechanical properties of Carbon Nanomembrane using wrinkling based metrology — •Himanshu P. Patel[1], Bernhard Alexander Glatz[1], Maria Kuellmer[2], Zian Tang[2], Andreas Winter[2], Andrey Turchanin[2], and Andreas Fery[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Dresden, Germany — [2]Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena, Germany — [3]Cluster of Excellence Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Germany

We demonstrate further development in application of wrinkling-based metrology (SIEBIMM) to evaluate the Young's modulus and mechanical properties for 2D materials. In this case we have used Carbon Nanomembranes (CNMs), a 1nm thin 2D molecular material with known mechanical properties. This work addresses critical issues in the sample preparation for this method related to the adhesion of 2D films on the substrate and volumetric swelling of the substrate during removal of the protective PMMA layer used for transfer of various 2D materials. The optimized procedure results subsequently in an easy to apply system for deriving immediate first results on the mechanical properties of 2D materials produced and transferred using a similar technique. We show the improved transfer of 2D materials to PDMS and further formation of wrinkle by application of strain. The wrinkle pattern is studied in situ using atomic force microscopy (AFM). Calculations using the SIEBIMM formula confirm the values reported in literature before.

HL 12.23 Mon 17:30 Poster E

Quantum Spin Hall Insulator Phase in Graphene/Bismuthene Quantum Well Heterostructure — Hamoon Fahrvandi[1], •Ebrahim Nadimi[1,2], and Michael Schreiber[2] — [1]Faculty of Electrical Engineering, Center for Computational Micro and Nanoelectronics, K. N. Toosi University of Technology, Tehran, Iran. — [2]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany.

Quantum spin Hall insulators (QSHI) have attracted much research interest due to their unique electronic properties. Time-reversal-symmetry-protected helical edge states provide dissipationless conductance at the boundaries of these two-dimensional (2D) systems. On the other hand, graphene another prominent 2D material, possesses just an ignorable QSHI phase with a small gap of about 1 meV. This is due to the weak spin-orbit coupling (SOC) in C atoms. In order to combine superior properties of graphene with unique electronic properties of novel QSHI, the idea of increasing SOC in graphene by proximity effect of a strong topological insulator has been proposed. This motivated us to investigate a vertical quantum well heterostructure of bismuthene-graphene-bismuthene (B-G-B) employing first-principles density-functional theory. We found that the proximity-enhanced SOC effect originating from bismuthene, leads to an enhancement in nontrivial topological nature of graphene. A weak van-der-Waals interaction in B-G-B heterostructure protects QSHI states with a sizable nontrivial gap. This structure can be a suitable candidate for realizing room temperature spintronic applications.

HL 12.24 Mon 17:30 Poster E

Coupled Organic Microcavities with Balanced Gain and Loss for Experimental Studies on Non-Hermitian Physics — •Karla Roszeitis[1], Markas Sudzius[1], Hartmut Fröb[1], Jan Carl Budich[2], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), TU Dresden, Germany — [2]Institute for Theoretical Physics, TU Dresden, Germany

Photonic systems are perfect model systems to experimentally investigate topological effects. One way to achieve topological non-trivial phases is to construct a parity-time symmetric system, comprising gain and loss, leading to non-hermitian terms in the corresponding Hamiltonian. In our experiments we realize a parity-time symmetric setup, consisting of two coupled organic microcavities. While one cavity contains an absorbing dye (loss cavity), the other can be pumped with a 532-nm laser (gain cavity). By thoroughly tuning the pump power as well as other parameters (e.g. coupling strength between the cavities) we achieve a parity-time symmetric system with pronounced modes in the visible regime.

We model the above mentioned system by a non-hermitian Hamiltonian $\mathcal{H}$ of the form $\mathcal{H} = \mathbf{d}(k) \cdot \sigma$. Here, $\mathbf{d} \in \mathbb{C}$ is a vector with complex components, k denotes the wave vector, and σ the vector of Pauli matrices. By the interplay between theoretical analysis of the Hamiltonian and recording of spectra we predict and explain the non-hermitian behaviour of the spectrum, in particular the mode splitting. Further research will address the ability of the gain cavity to exceed lasing threshold, steering the system into non-linear regime.

HL 12.25 Mon 17:30 Poster E

High frequency impact ionization and nonlinearity of photocurrent induced by intense terahertz radiation in HgTe-based quantum well structures — •Stefan Hubmann[1], Sebastian Gebert[1], Grigory Budkin[2], Vasily Belkov[2], Eugenius Ivchenko[2], Alexandr Dmitriev[2], Susanne Baumann[1], Maximilian Otteneder[1], Dimitry Kozlov[3], Nikolay Mikhailov[3], Sergey Dvoretsky[3], Ze-Don Kvon[3], and Sergey Ganichev[1] — [1]Terahertz Center, University of Regensburg, 93040 Regensburg, Germany — [2]Ioffe Institute, 194021 St. Petersburg, Russia — [3]Rzhanov Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

We report on a strong nonlinear behavior of photogalvanics and photoconductivity under excitation of HgTe quantum wells by intense terahertz radiation. The increasing radiation intensity causes an inversion of sign of the photocurrent and transition to its superlinear dependence on the intensity. The photoconductivity also shows a superlinear raise with the intensity. We show that the observed nonlinearities are caused by *light* impact ionization with a photon energy less than the band gap. The signature of this kind of impact ionization is that the angular radiation frequency $\omega = 2\pi f$ is much higher than the reciprocal momentum relaxation time. Thus, the impact ionization takes place solely because of collisions in the presence of a high-frequency electric field. The effect has been measured applying polarized radiation with f from 0.6 to 1.07 THz and intensities up to hundreds of kW/cm^2. We demonstrate that the impact ionization probability $W \propto \exp(-E_0^2/E^2)$, with the radiation electric field amplitude E and the field parameter E_0.

HL 12.26 Mon 17:30 Poster E

Phase-coherent transport and gating of top-down etched bulk-insulating topological insulator nanowires — •Dingxun Fan, Matthias Rössler, Oliver Breunig, Andrea Bliesener,

Gertjan Lippertz, Alexey Taskin, and Yoichi Ando — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany

A solid understanding of the phase-coherent transport properties of the surface states in quantum devices based on topological insulator (TI) nanowires is of fundamental importance for the exploration of various applicational concepts, e.g. Majorana-fermion-based topological quantum computing and spintronic devices. In general, a TI nanowire can be realized by natural growth, mechanical exfoliation or top-down etching from thin films. Despite the significant progress that has been achieved in the magnetotransport properties of the first two cases, which highlights the topological nature of quantized surface states, the investigation of thin-film-based nanowire devices is far from complete in revealing the role of topological surface states in transport.

Here we study the transport properties of top-gated $(Bi_{1-x}Sb_x)_2Te_3$ nanowires with width down to 100 nm realized by etching MBE-grown bulk-insulating thin films. Low temperature transport measurements show full gate tunability of both top and bottom surfaces. Mesoscopic transport phenomena including weak anti-localization, universal conductance fluctuations and Aharonov-Bohm oscillations are measured and compared both at and away from the Dirac point. The effect of local gating is also discussed.

HL 12.27 Mon 17:30 Poster E

Plasmonic modes in micro-ribbon arrays of topological insulators — •Philipp Warzanowski, Muhamad Saleh, Andrea Bliesener, Gertjan Lippertz, Yoichi Ando, and Markus Grüninger — Institute of Physics II, University of Cologne, Germany

The electronic surface states of topological insulators offer a rich playground to study unconventional plasmonic excitations in 2D by optical spectroscopy [1,2]. Spin-momentum locking leads to the emergence of the spin plasmon, a novel collective excitation carrying both spin and charge character. In thin films, spin plasmons on opposite surfaces interact via Coulomb interactions, yielding coupled modes which are either pure spin or pure charge modes [3]. The momentum q of the optically excited plasmon can be tuned by varying the periodicity of the micro-ribbon array. This work presents far-infrared measurements of micro-ribbon arrays of thin films of the topological insulator $Bi_{2-x}Sb_xTe_3$ grown on Al_2O_3. Plasmons hybridize with longitudinal phonons, resulting in excitations with a Fano lineshape [4]. By analysing the energy and lineshape as a function of the ribbon period, we study the character of the observed plasmonic excitations.

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[3] T. Stauber, J. Phys.: Condens. Matter 26, 123201 (2014).
[4] V. Giannini et al., Nano Lett. 11, 2835 (2011).

HL 12.28 Mon 17:30 Poster E

Exciton-polariton topological insulator — Sebastian Klembt[1], •Tristan H. Harder[1], Oleg A. Egorov[1], Karol Winkler[1], Rongchun Ge[2], Miguel A. Bandres[3], Monika Emmerling[1], Lukas Worschech[1], Timothy C. H. Liew[2], Moti Segev[3], Christian Schneider[1], and Sven Höfling[1,4] — [1]Technische Physik, Universität Würzburg, Germany — [2]School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore — [3]Physics Department and Solid State Institute, Technion, Israel — [4]School of Physics and Astronomy, University of St Andrews, UK

Topological insulators constitute a striking example of materials in which topological invariants are manifested in robustness against perturbations. Here, we demonstrate experimentally the first exciton-polariton topological insulator and as such the first symbiotic light-matter topological insulators. Exciton-polaritons arise from the strong coupling of quantum well excitons to microcavity photons. In polaritonic honeycomb lattices, we show the existence of a C = 2 Chern topological insulator, manifesting in a chiral, topologically protected edge mode.

HL 12.29 Mon 17:30 Poster E

Topological Hall effect in magnetically doped topological insulator thin films — •Gertjan Lippertz[1,2], Andrea Bliesener[1], Alexey Taskin[1], Lino Pereira[2], and Yoichi Ando[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]Instituut voor Kernen Stralingsfysica, KU Leuven, Belgium

Topological insulators (TIs) belong to a new class of quantum materials in which a strong spin-orbit coupling leads to a band inversion. Time-reversal symmetry (TRS), in turn, prevents the band gap from opening at the surface of the TI, leading to a protected metallic surface state.

Breaking TRS by magnetic doping opens an energy gap at the Dirac point on the top and bottom surface of the TI. Thin films of this kind of gapped topological insulator exhibit new quantum phenomena, including the quantum anomalous Hall effect (QAHE), where spontaneous magnetization leads to a dissipationless spin-polarised edge channel and a quantized Hall resistance of h/e^2.

Here we report on the observation of the topological Hall effect in V-doped $(Bi_xSb_{1-x})_2Te_3$ films grown by MBE and the possible existence of Skymions.

References:
[1] R. Yu et al., Science 329, 61-65 (2010)
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HL 12.30 Mon 17:30 Poster E

Topological surface states in α-Sn: from 3D Dirac semimetal to quasi-2D few-layer stanene — •Victor A. Rogalev[1], Johannes Jehn[1], Felix Reis[1], Florian Adler[1], Maximilian Bauernfeind[1], Jonas Erhardt[1], Liam B. Duffy[2], Thorsten Hesjedal[2], Moritz Hoesch[3], Gustav Bihlmayer[4], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut und Röntgen Center for Complex Materials Systems, Universität Würzburg, 97074 Würzburg, Germany — [2]Clarendon Laboratory, Physics Department, Oxford University, OX1 3PU, United Kingdom — [3]Diamond Light Source, Didcot, OX11 0DE, United Kingdom — [4]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich,52428 Jülich, Germany

We report on the TSS evolution in α-Sn films with different thickness and surface orientation, studied by angle-resolved photoemission. α-Sn films were grown epitaxially on InSb substrates (0.14% biaxial compressive strain) with (001)- and (111)-surface orientations, which renders a Dirac semimetal phase. For the (001)-oriented α-Sn films we observe quantum well effects in the electronic structure, while the Dirac point (DP) remains mainly unchanged down to $\sim$2.5 nm. The DP in (111)-oriented α-Sn was found to be 200 meV below the Fermi level for 10-nm-thick α-Sn film, which enabled us to observe the hybridization gap opening in TSS for lower α-Sn film thicknesses. The crossover to a quasi-2D few-layer stanene electronic structure is accompanied by a disappearance of the TSS spectral weight and a gap opening, in agreement with our DFT calculations of the electronic bandstructure.

HL 12.31 Mon 17:30 Poster E

Native point and layer defect in magnetically doped topological insulator multilayers — •Jakub Šebesta, Pavel Baláž, and Karel Carva — Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Ke Karlovu 5 121 16 Praha 2, Czech Republic

The effect of magnetic doping on surface states of topological insulators represents an interesting and highly debated problem, since magnetic field breaks the time-reversal symmetry guaranteeing surface band crossing. In reality several kinds of native defect could appear in these systems as well. Their inclusion allows to obtain a more realistic behavior as compared to the ideal one. Their presence could influence the size of a bulk and surface gap or the presence of ungapped surface states. The mutual interplay between defects is also important. In this work we focus on physical properties of magnetically doped well-know Bi_2Se_3 3D topological insulator [1] under the presence of native point and layer defects [2] treated by TB-LMTO+CPA within the surface Green's function approach. We show the impact of the mentioned defects on its bulk and surface band structure, especially on its gap size and magnetism related properties in the case of magnetic doping. The relations between occuring defects are discussed as well. Finally we try to compare exchange interactions leading to magnetic ordering as a function of composition.

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HL 12.32 Mon 17:30 Poster E

Boosting the Sensitivity and Selectivity of a Nanotube-Based NO_2 Gas Sensor: A First-Principles Investigation — Seyed Shahim Vedaei[1], •Ebrahim Nadimi[1,2], and Michael Schreiber[2] — [1]Faculty of Electrical Engineering, Center for Computational Micro and Nanoelectronics, K. N. Toosi University of Technology, Tehran, Iran. — [2]Institute of Physics, Chemnitz University of Technology,

09107 Chemnitz, Germany.

The sensing properties of carbon-nanotube (CNT) boron-nitride-nanotube (BNNT) heterostructures toward NO_2, O_2 and H_2O have been theoretically investigated applying first-principles density-function theory in combination with non-equilibrium Green's function formalism. The core idea is to change the current-flow mechanism in CNT to a quantum-mechanical tunneling process by introducing BNNT insulating layers within the CNT. Due to the strong sensitivity of the tunneling current to the barrier height and the influence of adsorbed agent on the position of the band edges in the BNNT layer a very high level of sensitivity is expected for the proposed device. The binding energies and current as well as the device sensitivity have been calculated for energetically favorable adsorption geometries of NO_2, O_2 and H_2O molecules. In general NO_2 and O_2 show higher sensitivity compared to H_2O molecule. In order to increase the selectivity, the application of a vertical electric field on the BNNT part of the device is suggested. It is shown that by collecting the signals at different vertical electric fields a very good selectivity can be expected toward NO_2, O_2 and H_2O gases.

HL 12.33 Mon 17:30 Poster E

Fabrication and properties of carbon-nanodot-based planar microcavities — •Lukas Trefflich[1], Frank Dissinger[2], Chris Sturm[1], Siegfried R. Waldvogel[2], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Felix-Bloch-Institute for Solid State Physics, Universität Leipzig, 04103 Leipzig — [2]Institute for Organic Chemistry, Johannes Gutenberg Universität Mainz, 55128 Mainz

We report about the growth and structural as well as optical properties of carbon-nanodot-based planar microcavities. The carbon nanodots made from citric acid emit bright light in the spectral range between 450 nm and 500 nm. By incorporating them in a microcavity and varying the cavitylayer thickness, it is possible to tune the emission wavelength of the device. We present the angularly and temporally resolved emission characteristic of the microcavity, as well as the dielectric function of the carbon-nanodot-containing cavity layer from the NIR to the UV spectral range. Furthermore, we explore their usage for possible laser and white light LEDs. White light LEDs usually contain rare-earth elements [1], which are less abundant and expensive. Carbon nanodots can be synthesized from environment-friendly substances like coffee, tea, grass and candle soot. [2] They are biocompatible [3] and photo-stable [4] and therefore promising alternatives for conventional LED designs. [1] H. Höppe, Angew. Chem., Int. Ed. 2009, 48 [2] Roy et al., Mater. Today, 2015, 18 [3] da Silva et al., Trends Anal. Chem., 2011, 30 [4] Sun et al., J. Am. Chem. Soc., 2006, 128

HL 12.34 Mon 17:30 Poster E

Redox and electrochemical doping of nanoscale semiconductors — •Klaus Eckstein, Florian Oberndorfer, and Tobias Hertel — Institute of Physical and Theoretical Chemistry, Am Hubland, Julius-Maximilians-University Würzburg, 97074 Würzburg

We report on recent advances with the spectroscopic characterization of doped semiconducting carbon nanotubes (SWNTs) using photoluminescence- and femtosecond time-resolved spectroscopies as well as IR-VIS absorption spectroscopy [1-2]. Our primary objective is to obtain an understanding of charge-induced modifications of exciton- and trion- photo- physics, that may eventually provide the basis for a quantitative spectroscopic assessment of carrier concentrations in doped nanotubes or other low-dimensional semiconductors.

Our investigations of electrochemically and redox-chemically doped SWNTs suggest that surplus carriers tend to be localized by their interaction with poorly screened counterions in the nanotube environment. These findings have important implications for several aspects related to the performance of doped nanoscale semiconductors in functional materials, specifically when it comes to charge and energy transport properties of these systems.

[1] H. Hartleb, F. Späth, T. Hertel, ACS Nano 9 (2015) 10461.

[2] K.H. Eckstein, H. Hartleb, M.M. Achsnich, F. Schöppler, T. Hertel, ACS Nano 11 (2017) 10401.

HL 12.35 Mon 17:30 Poster E

Improving the spin coherence of shallow nitrogen-vacancy centers (NVs) by CVD-diamond overgrowth — •Christoph Findler[1,2], Christian Osterkamp[1], Johannes Lang[1], Josef Souček[3], Milos Nesladek[3], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Ulm University, Albert-Einstein-Allee 11, D-89081 Ulm, Germany. — [2]Daimler AG, RD/EBT, HPC U028, Wilhelm-Runge-Str. 11, D-89081 Ulm, Germany. — [3]Institute for Materials Research (IMO), Hasselt University, Wetenschapspark 1, B-3590 Diepenbeek, Belgium.

The negatively charged nitrogen-vacancy center (NV) is a paramagnetic defect in diamond with long spin coherence times at room temperature. The spin-dependent fluorescence of the NV enables optical polarization, read-out and manipulation of single or ensembles of spins. For quantum technology applications like magnetic resonance imaging [1] and magnetic field sensing on the nanoscale [2] the NVs have to be close to the diamond's surface. To minimize the influence of near-surface noise and defects we combine two state-of-the-art NV production methods, namely plasma enhanced chemical vapor deposition (PECVD) [3] and nitrogen ion implantation with precise depth control [4]. We produce shallow NV centers by implantation into ^{12}C-enriched (100) diamond and overgrow then the NVs with a thin ^{12}C-enriched diamond capping layer using PECVD [4]. [1] T. Staudacher et al., Science 339, 561-563 (2013). [2] S. Schmitt et al., Science 356, 832-837 (2017). [3] C. Osterkamp et al., Appl. Phys. Lett. 106, 113109 (2015) [4] T. Staudacher et. al., Appl. Phys. Lett. 101, 212401 (2012)

HL 12.36 Mon 17:30 Poster E

Magnetic resonance of electrochemically fabricated carbon quantum dots — •Theresa Grünleitner[1], Jonathan Zerhoch[1], Martin Stutzmann[1], Martin S. Brandt[1], and Zhenhui Kang[2] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Garching, Germany — [2]Functional Nano & Soft Materials Laboratory (FUNSOM), Soochow University, Suzhou, China

Optically detected magnetic resonance is a unique technique to identify the microstructure of excited states leading to fluorescence. In this contribution, we apply this technique to investigate the origin of the luminescence in carbon-based nanoparticles synthesised via alkali-assisted electrochemical fabrication. ODMR measurements show broad structures up to about 600 G, which we assign to Pake doublets caused by triplet excitons. The assignment is corroborated by the observation of the corresponding half-field transitions. We discuss the correlation of this fine structure to the photoluminescence energy of the quantum dots and to the diameter of the particles.

HL 12.37 Mon 17:30 Poster E

Rydberg-like states in organic semiconductor rods — •Aswin Asaithambi[1], Daichi Okada[2], Guenther Prinz[1], Yohei Yamamoto[2], and Axel Lorke[1] — [1]Lotharstrasse 1, Faculty of Physics, CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Division of Material Science, Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Japan

The Organic semiconductor Borondipyrromethene (BODIPY) drawn much attention in recent years due to their advantageous photophysical properties. BODIPY molecules, under certain conditions, can be grown into crystalline rods [1]. Different growth methods result in BODIPY rods with different photo-emission wavelengths, for example green, orange or red [1].

In this contribution we show photo-luminescence (PL) spectra of green rods under 405nm laser excitation. The PL spectrum shows, besides a broad luminescence band, a set of peaks with energies that follows $E(n)=E_g-E_0/n^2$. E_g is the band gap and E_0 is the effective Rydberg constant that varies between different rods. Interestingly, PL line scans reveal that E_0 is constant within a single green rod and even in a serendipitously grown striped rods containing both red and green emitting regions.A slight decrease in the line width without a change in peak position was observed when lowering the temperature to 83K. The findings will be discussed using different models such as Rydberg excitons or charge complexes in the crystal.

[1] A. Asaithambi et al., JPC C DOI: 10.1021/acs.jpcc.8b09202

HL 12.38 Mon 17:30 Poster E

C8-BTBT air gap field-effect transistors — •Michael Bretschneider, Bernd Büchner, and Yulia Krupskaya — IFW Dresden, Germany

Despite the fact that organic semiconductors are already used to produce large scalable electronic devices, basic mechanisms of charge transport in these materials are not fully understood. The field-effect transistor is a common device to study charge transport in semiconductors by creating a conductive channel at the semiconductor/insulator interface. C8-BTBT is the workhorse of a new type of high hole mobility organic semiconductors. As a matter of fact there are several different mobilities reported in literature for comparable device struc-

tures of a C8-BTBT transistor. Electrical and mechanical distortion of the interface region caused by the solid dielectric cannot be excluded in these measurements, so that it remains unclear what the intrinsic mobility value of C8-BTBT is. With the help of an air gap field effect transistor we get rid of these distortions by using air/vacuum as an insulating layer between gate electrode and organic semiconductor. We investigate highly ordered films of C8-BTBT, grown by vapor phase transport. After the growth these films are flipped around and laminated with the upper surface on top of the air/vacuum gap stamp. In such a configuration it is possible to measure the current in the organic semiconductor which is not influenced by a gate dielectric. These measurements allow to get a closer look into the intrinsic transport behaviors of C8-BTBT.

HL 12.39 Mon 17:30 Poster E

Rubrene single-crystal based charge-transfer interfaces — •Bipasha Debnath[1], Eter Mgeladze[1], Alexey Popov[1], Yevhen Karpov[2], Anton Kiriy[2], Bernd Büchner[1], and Yulia Krupskaya[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden, 01069 Dresden — [2]Leibniz Institute of Polymer Research Dresden, 01069 Dresden

Organic materials based on small conjugated molecules are typically large gap semiconductors. However, it has been observed that if two of these materials are in direct contact, they can exhibit enhanced electrical conductivity at the interface. The conductivity is originated from the charge transfer between two constituent materials. Therefore, this conductivity can be used to study the charge transfer effects. One of the very good tools to investigate such phenomena is single-crystal charge-transfer interfaces. In this research work, we build and investigate Rubrene single-crystal based charge-transfer interface devices with new interesting acceptor materials such as fullerenes and hexacyano-[3]-radialene anion-radical material family. Here, we present different ways of fabricating these interface devices, i.e., thermal evaporation, drop-casting, spin coating, and shear coating as well as discuss the electrical properties of these interfaces. This work is financially supported by DFG KR 4364/4-1.

HL 12.40 Mon 17:30 Poster E

Comparing thickness dependence and transport properties of the organic semiconductors F_{16}CoPc and F_{16}CuPc — •Mareike Dunz, Karsten Rott, Jan Schmalhorst, and Günter Reiss — Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany

Nowadays, organic semiconductors are widely used in OLED and organic photovoltaic systems. However, organic field effect transistors cannot yet compete with silicon based technology as the search for high-mobility and air stable n-channel organic semiconductors goes on. Fluorinated metal phthalocyanines (F_{16}MPc) are considered to be promising candidates due to their high stability and easy synthesis but their carrier mobilities are insufficiently small. Understanding, how different metal center atoms influence the molecules' properties is a crucial step towards their applicability.

Hence, we prepared organic field effect transistors via thermal evaporation of F_{16}CuPc as well as F_{16}CoPc and investigated their thickness dependencies and transport properties at various temperatures. In situ measurements of the resistance allow for the detection of a thickness dependent source-drain current during the evaporation of the molecules and suggest a thinner conduction channel width for the F_{16}CoPc transistors. Furthermore, we show that oxygen dosing only worsens the performance of transistors with phthalocyanine thicknesses in the regime of the associated channel width, independent of the metal atom. Finally, as F_{16}CoPc features a magnetic center atom, first results of magnetic field dependent measurements are presented.

HL 12.41 Mon 17:30 Poster E

New insight into electronic excitations of metal phthalocyanines — •Louis Philip Doctor, Marco Naumann, Lukas Graf, Nikolay Kovbasa, and Martin Knupfer — IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany

We deposited thin films with a thickness of 120 nm, of copper-, zinc- and nickel-phthalocyanine on a KBr substrate in ultra-high vacuum, respectively. Afterwards these thin films underwent a phase transition to the β-phase. Furthermore the optical absorption spectra were measured at different temperatures down to 77 K. They show a drastic difference in the absorption of the initially evaporated α-phase compared to the β-phase in all optical regimes. The four peaks in the visible regime can be each assigned to a dipole transition element, which can be modelled by the extended double dipole approach. This model calculates the interaction between the two molecules in a metal-phthalocyanine dimer from crystallographic data. We added a distortion angle to model a momentum dependent dipole interaction. With electron-energy-loss-spectroscopy we are able to measure a momentum dependent excitation. Here again we see a different behaviour of the excitons in the α- and β-phase. The first excitation peak underwent a redshift for higher momentum transfer, whereas the second excitation peak virtually vanishes at the same time. This behaviour can be seen until a momentum transfer of 0.7 $Å^{-1}$. For higher momentum transfer this process seems to revert to the initial spectrum. This leads to the conclusion that excitons in metal-phthalocyanines have a negative dispersion with a minimum around 0.7 $Å^{-1}$.

HL 12.42 Mon 17:30 Poster E

Concept of multi-stage ballistic rectifiers — •Nina Niedworok and Ulrich Kunze — Electronic Materials and Nanoelectronics, Ruhr-Universität Bochum, 44780 Bochum, Germany

We analyze the behavior of input-current addition in a multi-stage ballistic rectifier implemented on Si/SiGe heterostructures. In a preceding work [1] we demonstrated a fundamental difference between two-stage ballistic rectifiers with large (740 nm) and small (340 nm) center-to-center separation between the current-injector pairs. While for large separation the output voltage V_{out} of both stages add up as $V_{out} = \alpha_1^2 I_{in1}^2 + \alpha_2^2 I_{in2}^2$ (where I_{in1}, I_{in2} are the input currents and α_1, α_2 denote the curvature coefficients) in closely-spaced stages the input currents are added leading to a characteristic which is accurately described by $V_{out} = (\alpha_1 I_{in1} + \alpha_2 I_{in2})^2$. More generally, this results in an excess voltage $V_{out}^{exc} = 2\beta\alpha_1\alpha_2 I_{in1} I_{in2}$, where β descibes the degree of overlap between the injected charge clouds of both stages, $0 \leq \beta \leq 1$. In the present work we present nanoscale geometries of multi-stage ballistic rectifiers which promise maximum excess voltage due to current addition. For n-stage rectifiers we present a model which describes the synergetic behavior. The aim of the work is to implement multi-stage ballistic rectifiers which show output voltages of technical relevance for high frequency applications with the smallest possible numbers of injectors on Si/SiGe heterostructures.

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HL 12.43 Mon 17:30 Poster E

Sign-alternating photoconductivity and magnetoresistance oscillations induced by terahertz radiation in HgTe quantum wells — •Maximilian Otteneder[1], Ivan Dmitriev[1,2], Susanne Candussio[1], Maxim Savchenko[3], Dmitry Kozlov[3], Vasily Bel'kov[2], Ze-Don Kvon[3], Nikolay Mikhailov[3], Sergey Dvoretsky[3], and Sergey Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Rzhanov Institute of Semiconductor Physics, Novosibirsk, Russia

We report on the observation of terahertz radiation induced photoconductivity and of terahertz analog of the microwave-induced resistance oscillations (MIRO) in HgTe quantum wells (QWs). The MIRO-like effect has been detected in 20 nm QWs with a mobility of 3×10^5 $cm^2/V\,s$. In other structures with QW widths ranging from 5 to 20 nm and lower mobility we observed an unconventional non-oscillatory photoconductivity signal which changes its sign upon magnetic field increase. In samples having Hall bar and Corbino geometries this results in a single and double change of the photoresponse sign, respectively. We show that within the bolometric mechanism these unusual features imply a non-monotonic behavior of the transport scattering rate, which should decrease (increase) with temperature for magnetic fields below (above) a certain value. This behavior is consistent with the results of dark magnetoresistivity measurements at different temperatures. Our experiments demonstrate that photoconductivity is a very sensitive probe of the temperature variations of the transport properties, even those that are hardly detectable using standard transport measurements.

HL 12.44 Mon 17:30 Poster E

Probing energy transfer in TMDC/organic heterostructures using Femtosecond Electron Diffraction — •Helene Seiler[1], Daniela Zahn[1], Soohyung Park[2], Thomas Vasileiadis[1], Ying-Peng Qi[1], Norbert Koch[2], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Department of Physics, Humboldt-Universität zu Berlin, Brook-Taylor-Straße 6, 12489 Berlin, Germany

Transition metal dichalcogenide (TMDC)/organic heterostructures have recently gained attention for their potential in opto-electronic ap-

plications. While first devices have been demonstrated, a microscopic understanding of the couplings within the sub-systems as well as between the sub-systems in the heterostructure is still lacking. Here we show how femtosecond electron diffraction can provide direct insights into these couplings using a MoS2/pentacene heterostructure as an example. Our measurements complement optical studies by revealing the energy relaxation pathways dominated by the participation of dark states and incoherent phonons, both not directly accessible with optics. The presented method is general and we expect that it can be applied to a wide range of heterostructures.

HL 12.45 Mon 17:30 Poster E

***In situ* study of the surface preparation of metamorphic GaAsP buffers for III-V-on-Si integration** — •Ammar Tummalieh, Agnieszka Paszuk, Oliver Supplie, Alexander Heinisch, Peter Kleinschmidt, and Thomas Hannappel — Institute for Physics, University of Technology, Ilmenau, Germany

Low defect $GaAs_{1-x}P_x$ graded buffers grown on Si enable highly efficient III-V-on-Si multi-junction solar cells. Here, $GaAs_{1-x}P_x$ graded buffers were grown by metalorganic chemical vapor phase deposition on GaP substrates to explore the possibility of *in situ* growth control. To this end, the GaAsP growth was monitored with reflection anisotropy spectroscopy (RAS). Ultra-high vacuum surface-sensitive methods were used to identify the surface reconstruction and chemical composition in dependence on the GaAsP stoichiometry and post-growth surface preparation routes. The strain relaxation of each layer was measured by high-resolution x-ray diffraction. We show that the As content of individual GaAsP layers can be quantified *in situ* during the growth by RAS: With increasing As supply, a peak close to the GaP E_1 critical point energy shifts towards GaAs E_1 at lower energy. The atomic structure of the GaAsP surfaces depends on the processing routes. GaAsP surfaces annealed at 500°C are V-rich whereas annealing at 700°C leads to Ga-rich surfaces. The preparation of the surfaces can be optimized *in situ* via their RAS fingerprints.

HL 12.46 Mon 17:30 Poster E

Heterostructures of 2D Materials and Organic Semiconductors for Ambipolar Field Effect Transistors — •Sirri Batuhan Kalkan[1], Henrik Hecht[1], Antony George[2], Andrey Turchanin[2,3], and Bert Nickel[1] — [1]Faculty of Physics and CeNS, Ludwig-Maximilians-Universität München, 80539 Munich, Germany — [2]Institute of Physical Chemistry, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany — [3]Jena Center for Soft Matter (JCSM), 07737 Jena, Germany

We investigated the electronic and optoelectronic properties of a MoS2 field effect transistor (FET) and a pentacene/MoS2 heterostructure as an ambipolar FET. Heterostructures are constituted by transferring a pentacene sheet on top of the MoS2 layer. This transfer is enabled by using low energy electron beams to crosslink the first couple of layers of pentacene increasing mechanical stability. Therefore, less defective surfaces are achievable in compared to photoresist or PMMA assisted transfer. In previous work, we introduced the technique of scanning photocurrent microscopy (SPCM) for spatially identifying defect sites within an OFET channel, as well as regions of low contacts. Now we employ this technique to the pentacene/MoS2 heterojunction. Here, pentacene serves as p-type and MoS2 as n-type semiconductor. Tuning the excitation wavelength allows to separate the contributions of the two semiconductor layers. Furthermore, the effect of surface adsorbates at ambient condition in comparison to N2 atmosphere is studied. Understanding how to operate at ambient conditions will be valuable for design of transistors and photodetectors.

HL 12.47 Mon 17:30 Poster E

Luminescence of indium residues after local droplet etching and thermal annealing on GaAs (111)A substrates — •Julian Ritzmann[1], Nandlal Sharma[2], Dirk Reuter[1,2], Henning Moldenhauer[3], Jörg Debus[3], Marc Portail[4], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Ruhr-Universität Bochum, D-44780 Bochum — [2]Universität Paderborn, D-33098 Paderborn — [3]Technische Universität Dortmund, D-44227 Dortmund — [4]CNRS-CRHEA, 06560 Valbonne, France

(111)A-oriented GaAs has proved as interesting substrate for the growth of nanostructures of high symmetry. GaAs quantum dots on (111)A-oriented substrates produced by droplet epitaxy, for example, exhibit reduced fine-structure splitting. However, these QDs are strongly distributed in size resulting in rather broad photoluminescence (PL) spectra. More uniform quantum dot ensembles are achieved by filling up nanoholes on (001)-oriented Al(Ga)As with GaAs. Ensemble PL inhomogeneous broadenings of less than 10 meV are realized. Nanoholes are generated via local droplet etching (LDE), a technique which is capable of alternating the substrate surface in various ways and to produce a wide spectrum of nanostructures. Our approach is to establish the LDE technique on (111)A-oriented substrates. Therefore, we present a study on different parameters for the LDE with indium droplets using atomic force microscopy, PL, micro-PL and cathodoluminescence. We discuss luminescent characteristics of indium residues which form InGaAs/GaAs heterostructures with the substrate material.

HL 12.48 Mon 17:30 Poster E

Ab-initio dynamics of highly excited amorphous graphene — Sergej Krylow, Othmane Benhayoun, •Lukas Nöding, Marie Kempkes, Tobias Zier, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Amorphous materials are ubiquitous in todays society. However, many properties of amorphous media are still not understood, and pose a challenge to theoretical and experimental methods. Here, we analyze the response of amorphous carbon to an intense ultrafast laser pulse using ab-initio molecular dynamics simulations and compare our results to recent XAS experiments performed at the EIS-TIMEX and Fermi beamlines. In particular, we observe in our simulations s ignificant changes in the electronic density of states upon laser excitation. These changes are consistent with the time-evolution of the absoprtion spectrum in experiments. We demonstrate that the changes of the electronic density of states are caused by a non-thermal melting of the system. This can be particularly observed in the time-evolution of the radial distribution function and the mean square displacements.

HL 12.49 Mon 17:30 Poster E

Time-dependent photo-conductivity in DCNQI radical ion salts — •Lisa Schraut-May[1], Sebastian Hammer[1], Florian Hüwe[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The material class of organic radical anion salts offers a wide range of attractive electronic and photo-physical properties. For instance, dicyanochinondiimine (DCNQI) coordinated by metal atoms is characterized by a low-dimensional metallic ground state at high temperatures which is transferred to an insulating state upon cooling to cryogenic temperatures. The corresponding metal-insulator Peierls transition is tunable by the chemical composition of the $Me(DCNQI)_2$ sidegroups and the choosen metal as well as by external parameters, e.g. the hydrostatic pressure. Moreover, it has been demonstrated that the Peierls transition can be initiated by photon absorption on picosecond time scales [1] which renders $Me(DCNQI)_2$ a model system for studying the time-dependent photo-switching between metallic and insulating ground state. We present studies on the transient photo-conductivity in $Cu(DCNQI)_2$ and $Li(DCNQI)_2$ single crystals. We characterize the photo-induced Peierls transition as function of sample temperature, incident light intensity as well as excitation wavelength. The variation of these parameters provides detailed insights in the mechanisms governing the phase transition and allows for evaluation of this material class for application as ultra-fast photo-switches.

[1] F. Karutz et al., Phys. Rev. Lett. 81 (1998) 143

HL 12.50 Mon 17:30 Poster E

Ab-Initio Electronic Structure Parameters of Thermoelectric Mg2X-Mg2Y (X,Y=Si,Ge,Sn) Substitutional Alloys — •Juan Guerra, Marcel Giar, Carsten Mahr, Michael Czerner, and Christian Heiliger — Justus Liebig University Giessen, Institut für Theoretische Physik, Giessen, Germany

There has been a wide interest in the Mg2X-Mg2Y substitutional alloys, between the isoelectronic X,Y=Si,Ge,Sn, for technological applications and fundamental research. We use the Bloch spectral density function, defined within the coherent potential approximation in the KKR method, to map an electronic band structure, to explore the electronic nature, and to extract parameters relevant for transport such as energy gaps and effective masses. We compute formation energy using total energy calculations, and we report deviations from Vegard's laws stronger when Y=Sn. General non-linear trends are reported in the measured quantitites, anisotropies in the effective masses, and the well-know convergence of the conduction bands at intermediate compositions of Mg2X_{1-x}Sn_x. We discuss the trends of our calculations,

and compare them with available experimental data.

HL 12.51 Mon 17:30 Poster E

DFT calculation of zero-field splitting for high-spin defects in solids — •Timur Biktagirov, Wolf Gero Schmidt, and Uwe Gerstmann — Universität Paderborn, Warburger str. 100, 33098 Paderborn, Germany

For high-spin point defects, the zero-field splitting (ZFS, also known as magnetic anisotropy) is one of the key spectroscopic signatures addressable by electron paramagnetic resonance (EPR). Due to the complex nature of the ZFS, its comprehensive interpretation often has to rely on a combination of the experiment and the first-principles theory [1,2]. We report on the recent progress in developing a general and efficient framework for density functional theory (DFT) based calculation of the ZFS in extended periodic systems implemented in the Quantum ESPRESSO software [3].

[1] S. Sinnecker, F. Neese, J. Phys. Chem. A 110, 12267-12275 (2006).
[2] F. Neese, J. Chem. Phys. 127, 164112 (2007).
[3] P. Giannozzi, et al., J. Phys Cond. Matter 29, 465901 (2017).

HL 12.52 Mon 17:30 Poster E

Phonon-mediated optical absorption of BAs using first principles simulation methods — •Ivona Bravić and Bartomeu Monserrat — TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Recently the semiconductor boron arsenide (BAs) was experimentally found to exhibit ultrahigh lattice thermal conductivity at room temperature. Its capability to dissipate heat has emerged much interest in the optoelectronics community, since the discovery of highly thermal conductive semiconductors is imperative to facilitate the performance of optoelectronic devices. Considering the design of materials for that application field, not only the thermal conductivity but also the interplay between optical properties and temperature needs to be studied rigorously.

Hence, we report a detailed first principles analysis of the phonon-assisted optical properties of BAs using semilocal and hybrid DFT methods. We combine the electronic structure simulation with phonon-calculations using finite differences and thermal lines for the study of temperature effects on the electronic bandstructure and optical absorption. We will present the underlying computational techniques and we will demonstrate how the electron-phonon interaction influences indirect absorption in BAs, and inherently defines the temperature dependence of the absorption spectrum. This case study will also serve as an example of how considering phonons proves invaluable to the design of novel conductor materials operating under realistic conditions.

HL 12.53 Mon 17:30 Poster E

Theoretical Description of Two-Dimensional Spectroscopy in a CdTe Quantum Dot doped with a Single Mn Ion — •Magnus Molitor, Tilmann Kuhn, and Doris Reiter — Institut für Festkörpertheorie, Wilhelm-Klemm-Straße 10, 48149 Münster

Quantum dots (QDs) doped with single Mn ions offer new opportunities in the field of spintronics. In these QDs the Mn ion behaves as a spin $M = \frac{5}{2}$ with six eigenstates $M_z = \pm\frac{5}{2}, \pm\frac{3}{2}, \pm\frac{1}{2}$ resulting in a photoluminescence (PL) spectrum consisting of six equally spaced lines even in the absence of a magnetic field. By increasing the magnetic field, states which are coupled by the exchange interaction are brought into resonance and multiple anticrossings are observed in the PL spectrum. However, using PL alone one cannot unambiguously distinguish if these resonances arise from different non-interacting states or from a coupled system. In contrast, two-dimensional (2D) four-wave mixing (FWM) spectroscopy allows us to disentangle involved spectra.

In this contribution we study two- and three-pulse excitations to probe the coherence and population dynamics of a QD doped with a single Mn ion. We model the system as an ensemble of QDs in different Mn spin states, whereby each member is comprised of a few-level system. Our study shows that 2D FWM is able to identify and investigate coherent coupling mechanisms between the excitonic excitations and the magnetic dopant in the QD.

HL 12.54 Mon 17:30 Poster E

OAM spectroscopy of fractional exciton polariton vortices — •Bernd Berger, Marius Kahlert, Daniel Schmidt, and Marc Assmann — Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany

Vortices are elementary excitations of exciton polariton condensates that receive significant attention. Their characteristic feature is a helical phase gradient $l \cdot 2\pi$ which translates into the orbital angular momentum (OAM) state of the emitted light field. We demonstrate a spectroscopic method which utilizes the technique of OAM sorting to transform the helical phase gradient of OAM states to a linear phase gradient. This enables the detection of the topological charge of exciton polartion vortices without an interferometric setup. We demonstrate that this method is not limited to integer topological charges, but also works for arbitrary fractional OAM states with phase rotations different from multiples of 2π, which is comparatively hard to do using interferometric techniques. In summary the method we present opens new ways in researching vortices in exciton polaritons especially tailored towards non-integer OAM states. We discuss the possibility of exciting fractional vortices in exciton polariton condensates and probing the time dynamics of complex polariton processes such as vortex decays or vortex switching.

HL 12.55 Mon 17:30 Poster E

PbWO4 ground- and excited-state properties from first-principles calculations — •Johannes Bilk, Kris Holtgrewe, Christof Dues, and Simone Sanna — Justus-Liebig-Universität Gießen, Institut für theoretische Physik, Heinrich-Buff-Ring 16, 35392 Gießen

The scheelite tungstate crystals such as PbWO4 feature peculiar optical properties, including the excitonic luminescence, which is based on the radiative transition within tetrahedral (WO4)2- group, where the exciton becomes autolocalised. In particular, lead tungstate is a dense, fast scintillator material, which is often employed in high end calorimetric detectors in high energy physics accelerators [1]. Unfortunately, our theoretical knowledge of the models is still poor if compared to its technological relevance. In order to fill this gap, we present a comprehensive theoretical investigation of the scheelite phase of PbWO4. The atomic and electronic structure as well as the optical absorption are calculated for from first principles. The structural and optical properties predicted from local and hybrid density functional theory are in good agreement with experiment and earlier theoretical work [2]. The electronic structure and optical response are found to be very sensitive to the computational approach. Exact-exchange calculations are found to open the band gap substantially by 1.07 eV. In contrast to earlier calculations, good agreement with the measured optical data is achieved.

[1] M. Nikl et al., J. Appl. Phys. 91, 5041 (2002). [2] Y. Zhang et al., Phys. Rev. B 57, 12738 (1998).

HL 12.56 Mon 17:30 Poster E

Linear and non-linear optical properties of adamantane-derived molecular clusters — •Christof Dues[1,2] and Simone Sanna[1,2] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Zentrum für Materialforschung (ZfM/LaMa), Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

A new class of molecular materials based on adamantane-type organotetrel chalcogenide clusters has recently attracted the attention of the scientific community due to its outstanding optical properties [1]. Depending on the composition (organic substiuents and tetrel atoms in the cluster core), these materials show either white-light generation or strong non-linear response upon IR radiation [2]. In order to determine the prerequisites for white light generation, different related clusters have been synthesized, which posses an additional ligand based on a coinage-metal atom [3]. To explore the optical response, we perform first-principles calculations within the density functional theory. Linear optical properties such as absorption and transmission are calculated basing on the electronic structure for both single molecules and molecular crystals. Furthermore, the frequency dependent non-linear optical response is estimated calculating the second harmonic coefficients $\chi^{(2)}_{\mathrm{SHG}}$ and the photoluminescence is modeled by constrained total energy calculations.

[1] N. W. Rosemann et al., Science **352**, 1301 (2016).
[2] N. W. Rosemann et al., J. Am. Chem. Soc. **138**, 16224 (2016).
[3] E. Dornsiepen et al., submitted (2018).

HL 12.57 Mon 17:30 Poster E

Voigt exceptional-points in anisotropic ZnO-based photonic structures — •Evgeny Krüger[1], Steffen Richter[1,2], Sebastian Henn[1], Heinrich-Gregor Zirnstein[3], Jesús Zúñiga-Pérez[4], Christiane Deparis[4], Lukas Trefflich[2], Chris Sturm[2], Bernd

Rosenow[3], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstr. 5, Leipzig — [2]ELI Beamlines/Fyzikální Ústav AV ČR, v.v.i., Za Radnicí 835, 25241 Dolní Břežany, Czech Republic — [3]Universität Leipzig, Institut für Theoretische Physik, Brüderstr. 16, 04103 Leipzig — [4]Université Côte d'Azur, CRHEA-CNRS, rue Bernard Gregóry, Valbonne, France

We report on exceptional points (EP) in planar ZnO-based microcavities with broken cylindrical symmetry, realized by inclining the optical axis of the uniaxial cavity layer to the mirror direction [1]. Such EPs represent non-Hermitian degeneracies in momentum space, related to a local complex-square-root topology of the resonator eigenenergies. The eigenmodes coalesce along these directions, yielding degeneracy in energy, broadening and polarization, the latter being either left or right circular. We prove the exceptional point nature experimentally and theoretically by monitoring the square-root topology around the EP and show how the occurrence and direction of EP can be controlled by the geometrical microcavity design.

[1] S. Richter et al., Phys. Rev. A 95, 023836 (2017)

HL 12.58 Mon 17:30 Poster E

Template-Assisted Fabrication of Spectrum-Programmable Superlattice Photonic Crystals for Efficient Solar Energy Harvesting — •Zhiqiang Zeng, Rui Xu, and Yong Lei — Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Superlattice photonic crystals (SPhCs) possess tremendous potentials as building blocks for high-performance solar thermal conversion systems because of their great flexibility in optical manipulation. To be as solar absorbers, the key points are to fabricate highly-ordered SPhCs in large scale and to realize spectrally-programmable selective light absorption spectra for different operational temperatures. In this work, wafer-scale nickel (Ni) SPhCs with excellent structural uniformity are fabricated by structurally replicating nanoporous alumina templates comprising two sets of nanopores (NPs) and nanoconcaves (NCs). Both self-aligned sets of NPs and NCs are simultaneously formed during the anodization of surface-patterned aluminum foils. The Ni SPhCs demonstrate omnidirectional polarization-independent selective light absorption spectra whose cutoff wavelength can be precisely programmed in the spectral range of 600 to 1500 nm. Below the cutoff wavelength all absorption efficiencies are enhanced to over 90% due to surface plasmon resonance and cavity resonance stemming from both NCs and NPs. All these advantages in optics and fabrication qualify Ni SPhCs as excellent candidates of solar absorbers for practical utilization.

HL 12.59 Mon 17:30 Poster E

A high power (11 W), tunable (1.45 - 1.65 μm) OPCPA for THz generation in organic crystals — •Ivanka Grguras, Torsten Golz, Michael Schulz, Jan Heye Buss, Robert Riedel, and Mark James Prandolini — Class 5 Photonics GmbH, Notkestraße 85, 22607 Hamburg, Germany

Owing to their high second-order nonlinear susceptibility, organic crystals have gained tremendous interest as THz generators. Recently high field THz generation in several organic crystal have been demonstrated [1-3]. Here we demonstrate a high power, tunable (1.45 - 1.65 μm) OPCPA with pulse duration of $<$ 36 fs and a repetition rate of 350 kHz for THz generation using organic crystals. To enhance the flexibility of this system, a second synchronized probe channel is available, delivering compressed pulses at 850 nm with $<$15 fs.

[1] M. Savoini *et al.*, THz Generation and Detection by Fluorenone Based Organic Crystals, ACS Photonics **5**, 671-677 (2018)
[2] A. Curcio *et. al.*, Terahertz-based retrieval of the spectral phase and amplitude of ultrashort laser pulses, Opt. Lett. **43**, 783 (2018)
[3] C. Vicario *et. al.*, Generation of 1.5-octave intense infrared pulses by nonlinear interactions in DAST crystal, J. Opt. **17**, 094005 (2015)

HL 12.60 Mon 17:30 Poster E

Structural, Energetic and Electronic Properties of Lanthanum and Fluorine Doped HfO_2/SiO_2 Gate Stack of MOSFETs — Arash Rahimi[1], •Ebrahim Nadimi[1,2], and Michael Schreiber[2] — [1]Faculty of Electrical Engineering, Center for Computational Micro and Nanoelectronics, K. N. Toosi University of Technology, Tehran, Iran. — [2]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany.

Aggressive down scaling of the dimensions of metal-oxide-semiconductor field-effect transistors requires the application of high-k gate dielectrics in order to keep the gate leakage current at an acceptable level. Among several candidates HfO_2-based high-k gate stacks have been shown to be the most promising solution. However, the high-k gate stacks suffer from high density of trap levels as well as difficulties in threshold voltage adjustment. Doping of the gate stack with different atoms such as La and F has been shown to improve the gate stack quality. We employed first-principles calculations to investigate different atomic structures for La and F doping agents and their interactions with oxygen vacancies in a SiO_2/HfO_2 gate dielectric stack. The formation energies are calculated for different configurations and the results show that the F atoms prefer to occupy the position of an oxygen vacancy, particularly at the SiO_2/HfO_2 interface. The energetically favored configuration for a La defect complex is also located at the HfO_2 layer close to the interface. F and La doping is shown to be applicable for the passivation of trap levels as well as for the adjustment of the threshold voltage.

HL 12.61 Mon 17:30 Poster E

From Hybrid Si Nanowire Transistors to Artificial Neurons — •Khrystyna Nych[1], Eunhye Baek[1,2], Taiuk Rim[3], Larysa Baraban[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden — [2]Center for Advancing Electronics Dresden — [3]Department of Electrical Engineering, Pohang University of Science and Technology

The rampant development of neuromorphic computing technologies inspired multiple alternatives to be presented - from complex CMOS circuits to novel circuit elements with external post-processing. Presently, both extensive training iterations and a large number of devices is necessary to enable error-free low pixel quantity image recognition tasks. We are striving to combine both strategies by proposing an electrically-controlled n-doped Si nanowire transistor on a silicon on insulator wafer as the computational means combined with an ionic silicate film spin-coated on top to emulate the biological function of the cell body. This cell body, also known as the soma, is responsible for processing multiple dendrite inputs and generating an electric signal, the action potential, which is sent through the axon to the next neuron. An electrical bias at the gate stimulates a polarization in the silicate film which modulates the nanowire current, depending on the voltage polarity. The time constants for charging and discharging the film depend on the concentration of ions in the sol-gel matrix, the intensity of the voltage applied, the frequency of the input pulses and the integration time.

HL 12.62 Mon 17:30 Poster E

Towards Dopant-free MOSFETs by Silicon Nitride Interface Engineering — •Lena Hellmich, Benjamin Richstein, and Joachim Knoch — Institut für Halbleitertechnik, RWTH Aachen University, Germany

Though doping enables conductivity in silicon and low contact resistances, and degenerate doping avoids carrier freeze out in low temperature applications. However, in deep nanoscale MOSFETs even at very high dopant concentrations only a few dopants reside in typical device volumes resulting in strong variability. Furthermore, the nanoscale size leads to deactivation of dopants increasing parasitic source/drain resistances. Thus, the replacement of dopants in nanoscale MOSFETs becomes more and more important. Our approach to replace the degenerate doping in source/drain (S/D)-contacts is a thin Fermi-Level-Depinning layer in the contact area between metal and silicon. In order to suppress the penetration of the metal wave function of S/D-contacts into the bandgap of silicon, very thin silicon nitride layers in sub-nm regime are fabricated. This thin insulating layer results in a Fermi-Level-Depinning; thus, the Schottky-barrier decreases, resulting in a lower contact resistance and suppression of ambipolar behavior. The metal work function, however, can be utilized to obtain N- or PMOS-like behavior. We fabricated dopant-free ohmic contacts are realized and characterized at room temperature and low temperatures. Besides, S/D-contacts with different metals and a thin silicon nitride layer to demonstrate unipolar behavior.

HL 12.63 Mon 17:30 Poster E

Temperature dependent electrical characteristics of a junction field effect transistor for cryogenic sub-attoampere charge detection — •Hüseyin Azazoglu, Paul Graf, Anahita Kavangary, Meike Flebbe, Kornelia Huba, Hermann Nienhaus, and Rolf Möller — Fakultät für Physik/Cenide, Universität

Duisburg-Essen, Germany

The electrical input and output characteristics of a commercial n-channel junction field effect transistor (JFET) is studied as a function of temperature in the range between 30 and 300K. As long as the charge carrier concentration is constant an increasing drain current is observed for reduced temperatures and low gate voltages. Using a constant mobility model for the device this behaviour can be explained with the higher electron mobility in the source-drain channel. For larger negative gate voltages a source-drain voltage is found at which the drain current is almost temperature independent. As soon as the charge carriers freeze out the input characteristics changes significantly due to the exponential decrease of the carrier concentration. The source-gate leakage current is measured through the entire temperature range in an open gate configuration. It decreases exponentially with lower temperatures by more than six orders of magnitude and reaches values of 0.01 attoampere below 160K. The result can be explained by the generation of electron-hole pairs in the depletion layer in agreement with the Shockley-Read-Hall model. As a consequence, JFETs at cryogenic temperatures can be employed as almost perfect charge detectors. Applications, e.g. in scanning probe potentiometry, are discussed.

HL 12.64 Mon 17:30 Poster E

Magnetotransport in nanostructured narrow-gap semiconductors — •Olivio Chiatti[1], Christian Riha[1], Johannes Boy[1], Aron Castro Martinez[1], Sergio Pezzini[2], Steffen Wiedmann[2], Christian Heyn[3], Wolfgang Hansen[3], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]High Field Magnet Laboratory, Radboud University Nijmegen, 6525ED Nijmegen, The Netherlands — [3]Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

Transport properties of low-dimensional electron systems can be effectively investigated by measurements in magnetic fields. We investigate the magnetotransport of semiconductor heterostructures and nanostructures with spin-orbit interaction (SOI), under the influence of in-plane and out-of-plane electric fields. We fabricated etched quantum point contacts (QPCs) embedded in Hall-bars with in-plane gates. The Hall-bars and the constrictions were defined by micro-laser photolithography and wet-chemical etching from an InGaAs/InAlAs quantum well with an InAs-inserted channel [1]. We have performed transport measurements at low temperatures in the combined QPC and Hall-bar structures in magnetic fields. We show that the gate-voltages can tune the filling-factor mismatch between bulk Hall-bar and QPC. We observe the crossover from reflection to transmission of the quantum Hall edge channels at the QPC and tunneling across the QPC between reflected edge states, which depends on the magnitude and direction of the in-plane electric field.

[1] Chiatti *et al.*, Appl. Phys. Lett. **106**, 052102 (2015).

HL 12.65 Mon 17:30 Poster E

1-D and 2-D Multi-Gate Devices: Tailoring the Potential Landscape on the Nanoscale — •Thomas Grap[1,2] and Joachim Knoch[1] — [1]Institute of Semiconductor Electronics, RWTH Aachen, Germany — [2]Peter Grünberg Institute 11, FZ Jülich, Germany

One-dimensional (1-D) materials such as nanowires (NW) and carbon nanotubes (CNT) as well as two-dimensional (2-D) materials like graphene and MoS_2 have attracted a great deal of attention as buildings blocks of future nanoelectronics systems. NWs and CNTs enable 1-D electronic transport. Considering sufficient gate control, devices based on quantum effects (e.g. quantum dots) can be formed within these nanostructures. Furthermore 2-D materials exhibit excellent electronic transport due to a very high electron mobility. In this study we examined the electronic transport properties of 1-D and 2-D nanostructures by utilizing a buried multi-gate architecture where a large number of gates are used (order of 10 and more). The multi-gate substrate allows to tailor the potential landscape of the nanostructures on the nanoscale. The influence of gate length and inter-gate distances as well as different top-dielectrics such as SiO_2 or Al_2O_3 are investigated. Various device configurations (e.g. RTD, superlattice-FET) are realized for different materials by applying appropriate voltages to the multi-gates. Measurements of field effect transistors at room temperature as well as low temperatures are shown.

HL 12.66 Mon 17:30 Poster E

Temperature-robust terahertz quantum cascade lasers using Ge/SiGe — Thomas Grange[1], •Stefan Birner[1], Giacomo Scalari[2], Giovanni Capellini[3], Douglas Paul[4], Monica De Seta[5], and Michele Virgilio[6] — [1]nextnano GmbH, 85748 Garching b. München, Germany — [2]Institute for Quantum Electronics, ETH Zurich, 8093 Zurich, Switzerland — [3]IHP GmbH, 15236 Frankfurt (Oder), Germany — [4]School of Engineering, University of Glasgow, G12 8LT Glasgow, UK — [5]Dipartimento di Scienze, Università di Roma Tre, 00146 Roma, Italy — [6]Dipartimento di Fisica "E. Fermi" Università di Pisa, 56127 Pisa, Italy

In the past 15 years, terahertz (THz) quantum cascade lasers have been developed using III-V materials. High output power has been demonstrated but the maximum temperature operation reported remains limited to 200 K. To achieve higher temperature operation, group IV semiconductors, thanks to their non-polar lattice, offer an interesting alternative. Nevertheless, group IV QCLs have not been demonstrated yet. Furthermore, an accurate theoretical prediction of their performance, in comparison with III-V systems is still lacking. In this work, we theoretically investigate transport and gain in n-type Ge/SiGe THz QCLs that leverage on L valley electrons using a nonequilibrium Green's functions (NEGF) model. The calculated maximum operation temperature in the Ge/SiGe QCL is found above room temperature. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 766719 - FLASH project.

HL 12.67 Mon 17:30 Poster E

Statistical studies of random silicon-germanium alloys using electronic structure calculations — •Willi Roscher[1,2,3], Florian Fuchs[1,2,3], Christian Wagner[1,2], Jörg Schuster[1,3], and Sibylle Gemming[1,2] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [3]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Random alloys are relevant for many applications. One example is silicon-germanium which is used for high frequency devices like heterojunction-bipolar transistors. We therefore investigate the electronic structure of $Si_{1-x}Ge_x$ alloys in the entire composition range $0 \leq x \leq 1$. For our study we use density functional theory in combination with bulk models of the alloys. To describe the band gap precisely we use the pseudopotential projector shift method as implemented in QuantumATK 18.06.

We perform a random generation of $Si_{1-x}Ge_x$ structures to get statistical distributions of the electronic properties. After optimizing the structure we evaluate the band structure by averaging equivalent directions in the Brillouin zone.

The mean of the band gap is in good agreement with experimental reference data. We also demonstrate wide variations of the band gap, which are in the range of about 10 %. Further properties, such as the lattice constant and the formation energy are studied as well. Finally, we investigated also the impact of additional carbon dopants in the silicon-germanium alloy.

HL 12.68 Mon 17:30 Poster E

Highly doped silicon for photonic and plasmonic applications — •Jura Rensberg, Kevin Wolf, Martin Hafermann, and Carsten Ronning — Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

For some time now, laser processing is a key technology in basic solid-state and material science research with a manifold of industrial applications, such as recrystallization and dopant activation in semiconductor industries. The basis of laser annealing is the deposition of large amounts of energy (a few J/cm^2) over very short time scales, which leads to surface layer melting followed by rapid resolidification. Pulsed laser annealing of ion-implanted silicon leads to the formation of supersaturated alloys with maximum substitutional dopant concentrations far greater than equilibrium solubility limits. Here, we show the optoelectronical properties of silicon doped to the laser-annealing-induced solubility limit with respect to photonic and plasmonic applications.

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Phosphorous doped Germanium nanowires — •Ahmad Echresh, Shima Jazavandi Ghamsari, Yordan M. Georgiev, and Lars Rebohle — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden Rossendorf, Bautzner Landstraße 400, D-01328 Dresden, Germany

Germanium (Ge) is a promising high mobility channel material for future nanoelectronic devices with a lower effective charge carrier mass than Silicon (Si) and higher electron and hole mobility. Materials with

high carrier mobility can enable increased integrated circuit functionality. Hence, Ge based nanoelectronic devices could offer improved performance at reduced power consumption compared to Si electronics. In this work, Ge nanowires were fabricated using electron beam lithography (EBL) and inductively coupled plasma (ICP) etching. Then ion beam implantation was used to introduce phosphorous (P) dopant atoms into the Ge nanowires. Afterwards, flash lamp annealing (FLA) was applied to recover the crystal structure of the Ge nanowires and activate the dopant atoms. Micro-Raman spectroscopy spectra showed that by increasing the fluence of ion implantation, the peak of optical phonon mode in Ge was broadened asymmetrically which shows that dopant atoms are electrically activated. Moreover, we are designing Hall Effect measurement configurations for single Ge nanowires to determine their mobility and carrier concentrations.

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Control of the photoluminescence of the silicon vacancy color center in 4H-silicon carbide by electric fields — •Lena Bergmann, Maximilian Rühl, Christian Ott, Michael Krieger, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Color centers in Silicon carbide (SiC) are promising candidates for novel quantum technology based on single photon sources [1]. In this study we report on the control of the photoluminescence (PL) of the silicon vacancy (V_{Si}) color center in 4H-SiC by electric fields at low temperatures. In particular, we monitored the ensemble PL depending on electric field strength and field direction. Structured epitaxial graphene is used as transparent electrodes at the surface to drive a static electric field. The V_{Si} color centers under investigation are created by proton implantation [2]. We observe a Stark splitting of the V_1' line of about 2.4 meV at a field strength of about 0.7 $\frac{V}{cm}$. In addition, the PL intensity of V_1' and V_1 changes in the presence of the field. In contrast, the V_1 line does not display any splitting.

[1] S. Castelletto *et. al.* Nature Materials 13, 151-156 (2013)
[2] M. Rühl *et. al.* Appl. Phys. Lett. 113, 122102 (2018)

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Optical Spin Injection in Silicon — •Eduard Sauter — Abt. Nanostrukturen Leibniz Universitaet Hannover

Silicon is a promising candidate for electron spin manipulation due to lack of nuclear spin of the 28 isotope and low spin orbit coupling due to inversion symmetry of the unit cell. I would like to present results of electron spin manipulation by circularly polarized light with energy close to the band gap in the NIR region. The observed decay of spin orientation with increasing magnetic field is an indicator for the spin lifetime of electrons.