HL 91: Poster IIIb (Joint session of DS and HL, organized by HL)

Topics: Oxides, Two-dimensional materials, Epitaxial growth

Time: Thursday 16:00–19:00 Location: Poster A

HL 91.1 Thu 16:00 Poster A

Formation of polar oxide thin films and interfaces: Insights from ab initio simulations — •Marc Landmann, Eva Rauls, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, Warburg Straße 100, 33098 Paderborn

The layer quality of heteroepitaxial ZnO films widely suffers from the lack of suitable substrate materials. In order to reduce the defect density of ZnO films, caused by the substantial lattice mismatch with common substrates, the introduction of MgO buffer layers turned out to be beneficial. [1-3] In addition, the buffer-layer approach facilitates the polarity control of ZnO films due to the formation of metastable rock-salt interlayers in the MgO buffer layer [2] as well as the ZnO films itself [3].

Here, we have studied the growth process of polar ZnO films with and without inclusion of MgO buffer layers of varying thicknesses and morphologies by state-of-the-art density functional theory calculations. Our results provide new insights into the fundamental growth dynamics of ZnO and MgO thin films and interfaces as well as the driving forces behind surface polarity selection.

[1] M. W. Cho et al., Semicond. Sci. Technol. 20, 13 (2005) [2] H. Kato et al., Appl. Phys. Lett. 84, 4562 (2004) [3] H. T. Yuan et al., J. Cryst. Growth 312, 263 (2010)

HL 91.2 Thu 16:00 Poster A

Elastic properties and strain-tuning of single-layer phosphorene — Daniel Midtvedt[1,2], Caio H. Lewenkopf[3], and •Alexander Croy[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Chalmers University of Technology, Göteborg, Sweden — [3]Universidade Federal Fluminense, Niterói, Brazil

Phosphorene (or black phosphorus) has attracted a lot of interest in recent times. Its unusual puckered structure leads to interesting anisotropic elastic and electronic properties with promising potential applications. Moreover, single-layer phosphorene is a direct semiconductor, which makes this material a candidate to be used in (opto)electronic devices. An important question in this context is the strain-dependence of the electronic band-gap.

We calculate the elastic properties of single-layer phosphorene using the valence-force model of Kaneta et al [1] and the approach given in [2], which accounts for the non-Bravais lattice structure of the material. Using a two-orbital tight-binding model [3], we study the strain-induced band-gap modification. We compare our results with recent *ab initio* calculations.

[1] C. Kaneta et al, Solid State Commun. **44**, 613 (1982).
[2] D. Midtvedt et al, arXiv:1509.02365.
[3] J.-W. Jiang and H. S. Park, Phys. Rev. **B91**, 235118 (2015).

HL 91.3 Thu 16:00 Poster A

Time-resolved photoluminescence spectroscopy on vanadium-(IV)oxide nanostructures — •Konstantin Neuhaus[1], Celina Hellmich[1], Nils Rosemann[1], Marc K. Dietrich[2], Peter J. Klar[2], Angelika Polity[2], and Sangam Chatterjee[1] — [1]) Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]) I. Physical Institute, Justus-Liebig University Giessen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany

Transitionmetal oxides show various intriguing phenomena which may be attributed to the complex interplay of various degrees of freedom such as electronic excitations, lattice vibration, and spin states of matter. Vanadium(IV)oxide for instance shows a metal-insulator transition at a lattice temperature of T_c=68°C which is accompanied by a change in the crystal structure. Here, we study the electro-optical response on VO_2 nanostructures. The microcrystalline samples are grown on various substrates by radio-frequency sputter-deposition and partially doped with Sr. The time-resolved photoluminescence characteristics are recorded for various lattice temperatures using a confocal streak-camera setup with high spatial resolution.

HL 91.4 Thu 16:00 Poster A

Magnetization dynamics of the Skyrmion cuprate Cu_2OSeO_3 — •Evgeniia Slivina[1], Prashant Padmanabhan[1], Rolf B. Versteeg[1], Petra Becker[2], and Paul H. M. van Loosdrecht[1] — [1]Physics Institute 2, University of Cologne, 50937 Cologne, Germany — [2]Institute for Crystallography, University of Cologne, 50939 Cologne, Germany

In chiral crystal structures, the competition between the Heisenberg exchange and Dzyaloshinskii-Moriya exchange leads to a helimagnetic ground state ordering. Interestingly, under the presence of an external magnetic field, the Zeeman interaction energy stabilizes the formation of topologically robust nanometer sized Skyrmion spin vortices. Recently, ultrafast inverse Faraday effect measurements have been used to address the fundamental magnetic relaxation processes of the Skyrmion lattice in the cuprate material Cu2OSeO3. Here, we extend upon these findings by employing the time-resolved magneto-optical Kerr effect (TR-MOKE). In addition, we investigate the time-domain dynamics of the weakly fluctuating regime at the boundary between the helical, conical, and paramagnetic phase.

HL 91.5 Thu 16:00 Poster A

Magnetization dynamics of the Skyrmion cuprate Cu_2OSeO_3 — •Evgeniia Slivina[1], Prashant Padmanabhan[1], Rolf B. Versteeg[1], Petra Becker[2], and Paul H. M. van Loosdrecht[1] — [1]Physics Institute 2, University of Cologne, 50937 Cologne, Germany — [2]Institute for Crystallography, University of Cologne, 50939 Cologne, Germany

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HL 91.6 Thu 16:00 Poster A

Nonlocal resistance in plasma hydrogenated graphene — •Tobias Völkl, Thomas Ebnet, Philipp Nagler, Tobias Korn, Christian Schüller, Dieter Weiss, and Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany

Plasma hydrogenation was used to modify monolayer graphene with the intent to increase the spin orbit coupling strength in graphene. Raman spectroscopy was employed to extract the defect concentration and to characterize the hydrogenation process. Further, the temperature dependence of the hydrogen desorption was examined. Electrical transport measurements on an as fabricated sample showed large nonlocal resistances. The high value of the nonlocal resistance and the absence of any inplane magnetic field dependence of this resistance indicate that this signal is not caused by the spin-Hall effect.

HL 91.7 Thu 16:00 Poster A

Population inversion in Landau-quantized graphene — •Samuel Brem[1], Florian Wendler[1], and Ermin Malic[2] — [1]Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, 10623 Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

In the presence of strong magnetic fields the linear band dispersion of graphene is quantized into non-equidistant Landau levels, which can be selectively excited and probed with circularly polarized light. The extraordinary arrangement of energy levels opens up the possibility to create a population inversion between optically coupled Landau levels of graphene [1]. This is an important prerequisite for the design of a highly tunable Landau level laser in the terahertz regime.

To prove that the predicted population inversion can be exploited to generate coherent laser light, a quantum optical investigation of

Landau-quantized graphene in a cavity is performed. Based on the density matrix formalism combined with a tight-binding approach, we study the ultrafast dynamics of Dirac electrons in a magnetic field coupled to the photons in an optical cavity. This approach allows us to address the question whether the emission of coherent laser light in a graphene-based Landau level laser is possible.

[1] F. Wendler, and E. Malic, Sci. Rep. 5:12646 (2015)

HL 91.8 Thu 16:00 Poster A

THz Photoconductivity of Epitaxial Graphene and the Possible Opening of a Bandgap — •Markus Göthlich[1], Cay-Christian Kalmbach[2], Mattias Kruskopf[2], Klaus Pierz[2], Franz-Josef Ahlers[2], and Andreas Hangleiter[1] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig, Mendelssohnstraße 2, D-38106 Braunschweig — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig

Due to it's Dirac like nature the Landau quantization in graphene is given by $E_n = \mathrm{sgn}(n)\sqrt{\Delta^2 + 2\hbar v_F^2 e\,|Bn|}$ with Landau level (LL) index n. This gives a nontrivial Shubnikov-de Haas-effect (SdH) depending on the magnetic field B and – different to conventional material systems – on the chemical potential. It also allows the observation of resonant inter-Landau-level transitions at different magnetic fields for a given transition energy as shown by Gusynin et al. (Phys. Rev. Lett. **98**, 157402 (2007)). Motivated by a simulation that shows that SdH measurements alone might not be able to distiguish between the effect of a bandgap and the effect of the chemical potential, we want to investigate here the influence of a possible opening of a band gap in epitaxial graphene on the cyclotron resonance. Therefore we use the change of the photoconductivity in the cyclotron resonance case in the SdH regime and in the THz spectral range ($\hbar\omega_{\mathrm{photon}} \approx 10\,\mathrm{meV}$) for epitaxial graphene on SiC. Our results can also be relevant for the detection of THz radiation by spectrally selective detectors based on cyclotron resonance in graphene.

HL 91.9 Thu 16:00 Poster A

Engineering the band structure and magnetism in edge corrugated zigzag graphene nanoribbons — •Prakash Parida[1] and Swapan K Pati[2] — [1]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Theoretical Sciences Unit, Jawaharlal Nehru Centre For Advanced Scientific Research, Bangalore 560064, India

Electronic structure and conductance properties of edge-corrugated zigzag graphene nanoribbons have been studied within the framework of p-orbital tight binding model with a mean field approximation to the Hubbard term. The results show that, both the band gap and magnetic moment increase with the depth of corrugation. Electric field modulates the carrier nature of mid-gap states to a great extent.

HL 91.10 Thu 16:00 Poster A

Towards biomedical sensing with chemically functionalized graphene FETs — •David Kaiser[1], Andreas Winter[1], Thomas Weimann[2], and Andrey Turchanin[1,3] — [1]Institute for Physical Chemistry, Friedrich Schiller University Jena, Lessingstr. 10, 07743 Jena, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [3]Jena Center for Soft Matter (JCSM), Philosophenweg 7, 07743 Jena, Germany

Graphene field-effect transistor (GFET) biosensors can intrinsically possess a very high sensitivity up to the fM level. However, this sensitivity is difficult to achieve in combination with high selectivity and specificity of the biomolecular binding events. Thus, covalent functionalization of GFETs results in impairing the electronic structure of graphene, which significantly reduces the device mobility. The functionalization of graphene via physisorption typically causes larger distances between the analyte and graphene plane, which reduces the number of charge carriers induced in graphene per binding event. Both effects reduce sensitivity of GFET biosensors. To overcome these problems, we employ ultrathin (~ 1 nm) dielectric carbon nanomembranes (CNMs) to chemically functionalize GFETs without impairing the electronic performance. A CNM is placed on top of graphene in the manner of all-carbon van der Waals heterostructures and acts as an analyte-specific electrochemical transducer [1]. We present and analyze the electronic characteristics of the fabricated hybrid CNM/graphene FET arrays.

[1] M. Woszczyna et al. Adv. Mater. 26, 4831 (2014).

HL 91.11 Thu 16:00 Poster A

Quasi-classical ballistic transport in graphene antidot superlattices — •George Datseris, Ragnar Fleischmann, and Theo Geisel — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany

Recent magneto-transport experiments have revealed that electrons in graphene can exhibit similar commensurability effects as those that have been observed in ballistic semiconductor devices. We therefore study quasi-classical models for transport in graphene monolayers patterned with antidot superlattices at magnetic fields below the quantum Hall regime. Using the first order approximation of the dispersion relation of graphene (i.e. the Dirac equation approximation) we reproduce the experimental findings. Progressing from this we explore parameter regions not yet studied in experiment and extend our model to include the quasi-classical dynamics generated by the second order approximation of the dispersion relation.

HL 91.12 Thu 16:00 Poster A

Magneto Transport Properties of Mesoscopic HOPG Graphite Flakes: Thickness Dependence — •Mahsa Zoraghi[1], José Barzola-Quiquia[1], Markus Stiller[1], Tobias Lühmann[2], and Pablo Esquinazi[1] — [1]Division for Superconductivity and Magnetism, Faculty of Physics and Earth Sciences, University of Leipzig, Linnestr. 5, D-04103, Germany — [2]Institute for Medicine Physics and Biophysics, University of Leipzig, 04107 Leipzig

The electrical transport properties of mesoscopic thin graphite flakes (HOPG) as function of temperature and magnetic field were investigated. Samples were measured in the range of 2 up to 310 K and magnetic fields of ±7 T. The temperature dependendent resistance $R(T)$ shows that samples thicker than ≈35 nm have metallic behavior and thinner samples show semiconducting-like behavior. The resistivity increases with decreasing sample thickness. We explained the $R(T)$ measurements using a model, which considers contributions in parallel. A contribution behaving like a 2DEG system formed at the interfaces of the crystals inside the sample; the other has a semiconducting behavior, which we attribute to the crystalline regions. The MR measurements show a thickness dependence, i.e. the change is reduced by reducing the thickness of the sample. Shubnikov de Haas (SdH) oscillations are more pronounced in thick samples, and show that the conductivity in our samples is dominated by two types of carriers. The results indicate that transport properties of bulk graphite are not intrinsic and depend on the interfaces. Raman results reveal that all of the samples have the same structural quality as of bulk HOPG.

HL 91.13 Thu 16:00 Poster A

The substrate dependence of localizing excitons in WSe2 monolayers — •Jhih-Sian Tu[1], Sven Borghardt[1], Florian Winkler[2], Detlev Grutzmacher[1], and Beata Kardynal[1] — [1]PGI-9, Forschungszentrum Juelich, Juelich, Germany — [2]ER-C, Forschungszentrum Juelich, Juelich, Germany

Monolayer transition-metal dichalcogenides (TMDs) have become new building blocks for two-dimensional (2D) heterestructures which are composed of monolayers of different materials bound with Van der Waals forces. In this study, the photoluminescence (PL) of WSe2 monolayers (ML) is compared with that of hexagonal-boron nitride (hBN)/WSe2 ML/hBN heterostructures. The samples were prepared by PDMS dry transfer of WSe2 MLs on target substrates (SiO2 or hBN). The PL measurements showed that encapsulation leads to a suppression of the free exciton emission and to a shift of the exciton emission energy. An impurity band emission, although present in all sample geometries, is also strongly modified by the encapsulation. It is present across the whole sample and takes a form of a set of sharp emission lines in wide wavelength range. These sharp emission lines are linearly polarized as in the case of the emission from the localized states in WSe2 on SiO2 or on hBN. Variations in geometries of measured samples allow the analysis of the data in terms of influence of external impurities, intrinsic defects and a surface strain caused by hBN encapsulation. We discuss the substrate choice for the control of photoluminescence from localized states in WSe2 ML.

HL 91.14 Thu 16:00 Poster A

Ab initio elasticity of Ga_2O_3 in the α and β phase — •Konstantin Lion, Dmitrii Nabok, Pasquale Pavone, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin D-12489 Berlin

The transparent conducting oxide Ga_2O_3 has a wide band gap of about

4.4 - 4.8 eV. It is a very promising candidate in a number of applications, such as transparent electrodes for UV optoelectronic devices, semiconducting lasers and transparent electrodes in solar cells. Depending on the preparation, Ga_2O_3 can crystallize in 5 different structures, among them the monoclinic β and the hexagonal α phase. The structural and elastic properties of these phases are investigated from first principles using the full-potential all-electron code `exciting` [1]. The calculated lattice parameters are in good agreement with experimental and previously reported theoretical results. Second-order elastic constants of both phases are calculated using the tool `ElaStic` [2]. Furthermore the stability of these 2 phases is investigated by applying stability criteria, such as the Born criteria.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] R. Golesorkhtabar *et al.*, Comp. Phys. Commun. **184**, 1861 (2013).

HL 91.15 Thu 16:00 Poster A

PAMBE-Growth of SnO_2 — •Max Kracht, Alexander Karg, Jie Jiang, Jörg Schörmann, and Martin Eickhoff — I. Physikalisches Institut der JLU Gießen, Heinrich-Buff-Ring 16, D-35392 Gießen

The application of tin dioxide (SnO_2) as gas sensitive material or highly doped as a transparent conducting oxide has been investigated in detail. To further increase the application range of this non-toxic, chemically stable material and to gain further knowledge of the basic material properties, single crystalline thin films are required.

Plasma-assisted molecular beam epitaxy is a well established method to gain high quality crystalline films. Therefore SnO_2 thin films were grown by PAMBE on r-plane sapphire substrates. The influence of different growth parameters like substrate temperature or tin beam equivalent pressure on the structural and electrical film characteristics are investigated using high resolution X-ray diffraction (HRXRD), scanning electron microscopy (SEM), atomic force microscopy (AFM) and Hall measurements.

HL 91.16 Thu 16:00 Poster A

Group-IV doping of ion-beam sputtered Ga_2O_3 — •Philipp Schurig, Martin Becker, Fabian Michel, Angelika Polity, and Martin Eickhoff — 1st Physics Institute, Justus-Liebig-University Giessen, Giessen, Germany

For the last years the interest in transparent conductive materials stayed at a high level due to possible applications in the field of (opto-)electronics, for example as photoresistors/-diodes, high temperature sensors and solar cells. The thermodynamically most stable oxide of gallium, β-gallium oxide, has monoclinic crystal structure and a band gap of around 4.9 eV.

One requirement for the usage in electronics is a controllable carrier concentration, achievable by n-type doping with suitable elements as there are Sn, Si and Ge. With Ion-Beam-Sputtering from a Ga_2O_3 target Sn, Si and Ge doped samples were prepared. The substrate holder was heated to 650 °C during deposition and c-sapphire and quartz substrates were used.

Transmittance, X-Ray-Diffraction, Energy Dispersive X-Ray Spectroscopy and Scanning Electron Microscopy measurements were performed to characterize the deposited layers after deposition and to investigate the effect of a post-deposition anneal at temperatures of 1000 °C and above in oxidizing atmosphere. An improvement of the structural properties and a blue-shift of the optical absorption edge were observed.

HL 91.17 Thu 16:00 Poster A

An X-ray photoelectron spectroscopy (XPS) study on NiO/SnO_2 and SnO/SnO_2 heterojunctions — •Fabian Michel, Benedikt Kramm, Martin Becker, Robert Hamann, Angelika Polity, Detlev M. Hofmann, and Martin Eickhoff — Justus-Liebig Universität Giessen, Germany

The energy band diagrams of different pn-heterojunctions were evaluated by X-ray photoelectron spectroscopy. The heterojunctions were fabricated by ion beam sputtering. The valence band and conduction band discontinuities of NiO/SnO_2 and SnO/SnO_2 were investigated using the common method of E.A. Kraut[1] and J.R. Waldrop[2] considering the position of the different core level signals and especially the related energy difference in the vicinity of the heterointerface. Using depth profiling via in situ Ar+ ion etching we made a qualitative analysis of the interfacial chemical state by estimating the modified Auger parameter and the relative concentrations of the photoelectron signals. We also investigated the challenging Ni 2p signal by decomposing the line structure and the satellite structure. Results will be discussed with respect to other metal oxide heterojunctions.

[1] Kraut, E. A.; Grant, R. W.; Waldrop, J. R. und Kowalczyk, S. P., Semiconductor core-level to valence-band maximum binding-energy differences: Precise determination by x-ray photoelectron spectroscopy. Phys. Rev. B, Aug. 1983, 28(4):1965
[2] Waldrop, J. R. und Grant, R. W., Measurement of AlN/GaN (0001) heterojunction band offsets by x-ray photoemission spectroscopy. Applied Physics Letters, 1996, 68(20):28792881

HL 91.18 Thu 16:00 Poster A

Energy Band Alignment of Novel p-type Transparent Conducting Oxides on Indium Tin Oxide — Emma Norton, Leo Farrell, Daragh Mullarkey, Igor Shvets, and •Karsten Fleischer — School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College, University of Dublin, Dublin 2, Ireland

Thin films of p-type Cr_2O_3:Mg have been produced by Molecular Beam Epitaxy (MBE) as well as amorphous, copper deficient p-type Cu_xCrO_2 deposited by a low temperature solution based method (spray pyrolysis). These thin films are deposited on top of commercial n-type Indium Tin Oxide substrate to produce transparent pn junctions. The band alignment of these two interfaces is studied using X-ray Photoelectron Spectroscopy (XPS) and Ultra Violet Photoelectron Spectroscopy (UPS). An estimate of the band discontinuities at the interfaces of ITO/Cr_2O_3:Mg and ITO/a-Cu_xCrO_2 are given. An emphasis is given to the fact that the Fermi level and work function position for both Cr_2O_3:Mg and a-Cu_xCrO_2 show changes with surface preparation and surface termination.

HL 91.19 Thu 16:00 Poster A

Noise spectroscopy on In_2O_3 films — •Bonito Thielert[1], Fariba Hatami[1], W. Ted Masselink[1], Oliver Bierwagen[2], and James S. Speck[3] — [1]Humboldt-Universität zu Berlin, Inst. für Physik, Newtonstr. 15, 12489 Berlin — [2]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin — [3]Materials Department, University of California, Santa Barbara, USA

How good is the quality of In_2O_3 layers? In order to answer this question, several In_2O_3 samples were grown using molecular-beam epitaxy on Y-stabilized ZrO_2(001) wafers. Mg-, Zn- and unintentionally doped samples were after growth thermally annealed in vacuum and in oxygen environment to change the compensating point defect concentration. The influence of doping and annealing of the electronic properties and the material quality were investigated by noise spectroscopy and Hall measurements. Our results show that most samples annealed in vacuum have 1/f noise with higher magnitude compared to samples annealed in oxygen environment. The estimated Hooge-factor [1] was between 10^{-2} and 10^{2} depending on the type of the doping and the annealing conditions. The Mg-doped sample annealed in oxygen environment has the lowest Hooge-factor of 10^{-2}. The value is more than one order lower than the reported value for the amorphous In_2O_3 [2]. The Sn-doped sample annealed in vacuum, on the other hand, has the highest Hooge-factor. The Hooge-factor will be qualitatively correlated to conductivity and the concentration of dopants and point defects.

[1] F. N. Hooge, Physica (Amsterdam) 60, 130 (1972) [2] R. E. Johanson, and S.O. Kasap, J. Vac. Sci. Technol. A 20, 1027 (2002)