DS 22: 2D semiconductors and van der Waals heterostructures V (joint session HL/DS/O)

Time: Wednesday 9:30–13:00 Location: POT 81

DS 22.1 Wed 9:30 POT 81

Impurity effects in graphene: resonances, localized states and Mott-transitions — Yuriy G. Pogorelov[1], •Denis Kochan[2], and Vadim M. Loktev[3] — [1]1IFIMUP-IN, Departamento de Física, Universidade do Porto, Porto, Portugal — [2]Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany — [3]N.N. Bogolyubov Institute of Theoretical Physics, NAS of Ukraine, Kyiv, Ukraine

Impurities modify electronic spectrum of graphene in several ways. For example, they can shift charge neutrality point, tilt the Fermi level, open spectral (quasi)gaps, form resonances, and localized states.

In the presentation we discuss formation of resonances, and localized states in graphene for Anderson-like impurities (Hydrogen, Copper, Fluorine) in top, bridge and hollow positions. Particularly, we focus on spectral transition between resonant and localized states, and Mott mobility edges, tracing dependencies on graphene Fermi energy, concentration of impurities, their sub-lattices distribution, and impurity hybridization strength.

Employing the group expansion of the Green's functions we calculated reconstructed band structure of graphene hosting Anderson impurities. Applying Ioffe-Regel-Mott criterion, we obtained system-specific critical concentrations at which system undergoes resonance-to-bound-state transition.

DS 22.2 Wed 9:45 POT 81

Twisted Bilayer Graphene Produced by Atomic Force Microscopy Techniques — •Lina Bockhorn, Lucas Gnörich, Johannes C. Rode, Christopher Belke, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The electronic properties of bilayer graphene strongly depend on relative orientation of the two atomic lattices. The rotational mismatch between both layers opens up a whole new field of rich physics, especially around the magic angle.
Twisted bilayer graphene can be obtained by different methods. Here, we use atomic force microscopy techniques to generate twisted bilayer graphene. A diagonal cut is applied at high contact force through a monolayer graphene. Several folds spread from the newly created edge. The self-assembled twisted bilayer graphene is separated in folds with one or two rips.
We estimate the relative orientation of twisted bilayer graphene which is prepared by folding monolayer graphene [1, 2, 3].

[1] H. Schmidt, J. C. Rode, D. Smirnov, R.J. Haug,
Nature Communications 5, 5742 (2014)
[2] J. C. Rode, D. Smirnov, C. Belke, H. Schmidt, R.J. Haug,
ANNALEN DER PHYSIK 529 (11), 1700025 (2017)
[3] J. C. Rode, D. Zhai, C. Belke, S. J. Hong, H. Schmidt, N. Sandler, R. J. Haug, 2D Materials, 6(1), 015021 (2019)

DS 22.3 Wed 10:00 POT 81

Magneto-Raman Spectroscopy for Probing Electron-Phonon and Electron-Electron Interactions in Graphene — •Jens Sonntag[1,2], Sven Reichardt[1,3], Ludger Wirtz[3], Mikhail Katsnelson[4], Bernd Beschoten[1], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — [3]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [4]Radboud University, Institute for Molecules and Materials, Nijmegen, Netherlands

We present charge carrier density-dependent magneto-Raman spectroscopy measurements on suspended graphene and hBN/graphene heterostructures to investigate electron-phonon and electron-electron interactions, both without applied magnetic field and within the quantum Hall regime. Strikingly, at $B = 0\,\mathrm{T}$ we do not observe the expected strong renormalization of the G-mode energy as a function of charge carrier density n. We identify Laser induced heating and a limited electron-hole lifetime as possible origins.
Utilizing gate-tunable magneto-phonon resonances, we extract the charge carrier density-dependence of the Landau level transition energies and the associated effective Fermi velocity v_F. In contrast to the logarithmic divergence of v_F at zero magnetic field, we find a piecewise linear scaling of v_F as a function of n, due to a magnetic field-induced suppression of the long-range Coulomb interaction. Furthermore, we can estimate the excitonic correction to the energies of the Landau level transistions to $\approx 6\,\mathrm{meV}$.

DS 22.4 Wed 10:15 POT 81

Tip-enhanced Raman spectroscopy combined with other Scanning Probe Microscopy Methods: Focus on 2D Materials — •Jana Kalbacova[1], Marc Chaigneau[2], and Andrey Krayev[3] — [1]HORIBA Jobin Yvon GmbH, Germany — [2]HORIBA Scientific, France — [3]HORIBA Scientific, USA

New two dimensional materials are on the rise. After the wonder material graphene, new materials such as MoS2, MoSe2, WSe2 have an intrinsic bandgap and as such are opening new doors for semiconductor applications. Raman spectroscopy offers information on the chemical structure of materials but cannot provide information on the electronic properties such as surface potential or photocurrent of our sample. Co-localized measurements combining scanning probe microscopy (SPM) with Raman spectroscopy can already bring a wealth of information; however, further improvements can be obtained by a tip that will act as an antenna and amplify the Raman signal and thus breaking the diffraction limit in a method called Tip-enhanced Raman spectroscopy (TERS). Typically spatial resolution of 10 - 20 nm can be achieved. In this contribution, we investigate different 2D materials by a combination of TERS, tip-enhanced photoluminescence, Kelvin probe microscopy, and other SPM methods to show very locally for example doping variations or defects that would otherwise go unnoticed with other macro- and microscopic techniques.

DS 22.5 Wed 10:30 POT 81

Edge photogalvanic effect driven by optical alignment in bi-layer graphene — •Susanne Candussio[1], Mikhail V. Durnev[2], Jun Yin[3], Artem Mishchenko[3], Helene Plank[1], Vasily V. Bel'kov[2], Sergey A. Tarasenko[2], Vladimir Fal'ko[3], and Sergey D. Ganichev[1] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]Ioffe Institute, 194021 St. Petersburg, Russia — [3]University of Manchester, Manchester M13 9PL, UK

We report on the observation of the edge electric current excited in bi-layer graphene by terahertz laser radiation. We show that the current generation belongs to the class of second order in electric field phenomena and is controlled by the orientation of the THz electric field polarization plane. Application of a magnetic field normal to the graphene plane leads to a phase shift in the polarization dependence. In strong magnetic field the current exhibit 1/B-magnetooscillations with a period consistent with that of the Shubnikov-de-Haas effect and amplitude by an order of magnitude large as compared to the current at zero field measured under the same conditions. The developed microscopic theory shows that the current is formed in the edges vicinity limited by the mean-free path and originates from optical alignment of free carriers and scattering at the edges, which naturally break the P-symmetry. The observed magnetooscillations of the photocurrent are attributed to the formation of the Landau levels.

DS 22.6 Wed 10:45 POT 81

Electronic Properties of Two-Dimensional $ZrSe_3$-Films — •Lars Thole[1], Christopher Belke[1], Sonja Locmelis[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

The family of 2d materials offers a big variety of different material classes [1]. This includes the transition metal trichalcogenides (TMTC) of the form MX_3, where M is a transition metal and X is a chalcogen [2, 3]. Here we exfoliated $ZrSe_3$ into thin films and contacted them with electron beam lithography. These thin flakes were investigated by means of optical microscopy, atomic force microscopy and electrical measurements. During this, it was shown that the material degrades in ambient condition. Furthermore, an activation energy of about 0.6 eV was measured. Inducing charge carriers showed the samples to be n-doped semiconductors. Finally, a mean free path for the bulk material was determined.

[1] A. K. Geim et al., Nature, 499, 419-425 (2013).

[2] J. O. Island et al., 2D Materials, 4, 0220033 (2017).
[3] J. Dai et al., WIREs Comput. Mol. Sci., 6, 211-222 (2016).

30 min. break

DS 22.7 Wed 11:30 POT 81

ultraviolet photodetectors based on mechanically exfoliated few-layer FePS3 and ZnO quantum dots with high responsivity — •Juanmei Duan[1,2], Liang Hu[3], Yujia Zeng[3], Manfred Helm[1,2], Shengqiang Zhou[1], and Slawomir Prucnal[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany — [2]Technische Universität Dresden, D-01062 Dresden, Germany — [3]College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, P. R. China

Metal-phosphorus-trichalcogenides (MPTs), FePS3, are newly developed 2D wide-bandgap semiconductors and have been proposed as excellent candidates for ultraviolet (UV) optoelectronics. In this work, few-layer FePS3/ZnO quantum dots heterojunction were studied with Transmission electron microscopy (TEM), scanning electron microscope (SEM), X-ray photoelectron spectroscopy (XPS), and Raman measurement. The photoresponse characteristic of UV detectors based on FePS3/ZnO were investigated under 365nm, 405nm illumination and bias voltages. The high photoresponse property paves the way for the further development of 2D MPTs/ZnO quantum dots in high-performance UV photodetectors.

DS 22.8 Wed 11:45 POT 81

Selectively grown Topological Insulator Nanodevices — •Daniel Rosenbach[1], Abdur Rehman Jalil[1], Jonas Kölzer[1], Nico Oellers[1], Michael Schleenvoigt[1], Tobias Werner Schmitt[2], Peter Schüffelgen[1], Gregor Mussler[1], Hans Lüth[1], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Peter Grünberg Institut (PGI-9) and JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich, 52425 Jülich, German — [2]JARA-FIT Institute Green IT, RWTH Aachen University, 52062 Aachen, Germany

1-dimensional topological insulator nanoribbons in close proximity to elemental superconductors can be utilized to create localized Majorana modes for topological quantum computation architectures. We employ a selective area growth method using molecular beam epitaxy in order to define topological insulator nanodevices without harmful post processing steps. Using the transmission line method the interface of Bi_2Te_3 nanorribons towards ex situ applied Ti/Au contacts is probed at low temperatures. Furthermore, magnetotransport measurements on nano-Hallbars of down to 50 nm wide Bi_2Te_3 nanoribbons show indications of highly mobile charge carriers originating from 2-dimensional, topological surfaces. Finally, making use of a stencil mask on-chip, elemental superconductors like Nb and Al are deposited to define in situ, lateral topological Josephson junctions. Superconducting properties of proximitized topological nanoribbons are presented and discussed.

DS 22.9 Wed 12:00 POT 81

Investigation of one-dimensional materials — •Hadeel Moustafa, Peter Larsen, Morten Gjerding, and Karsten Jacobsen — Technical University of Denmark (DTU), department of physics.

1D materials are an interesting subset of materials with promising applications in batteries, photonic crystals and as electronic interconnects. 1D materials also present the possibility of combining them with other 1D materials or higher dimensional materials to create new hetero-structures with novel physical properties. Another potential application could be in heterogeneous catalysis, where the restricted geometry of 1D materials might lead to new types of atomic sites with different chemical characteristics. We identify potential 1D materials through a screening procedure applied to the ICSD and the COD. We employ the dimensionality scoring parameter defined in ref [1], which is based exclusively on the atomic geometry. The algorithm extract one-dimensional components from periodic three-dimensional crystals. So far around 300 compounds have been studied. Their basic properties like atomic structure, stability (heat of formation and convex hull), band structure, density of states and work function have been calculated. They are furthermore characterized using symmetry and grouped together using a clustering algorithm based on the root-mean-square-distance. In the future we expect to construct new potential 1D materials by element substitution in the constructed database. [1] http://doi.org/10.1103/PhysRevMaterials.3.03400.

DS 22.10 Wed 12:15 POT 81

Proximity exchange effects in excitons of TMDC/ferromagnet van der Waals heterostructures — •Paulo E. Faria Junior, Klaus Zollner, and Jaroslav Fabian — Universität Regensburg, Germany

Proximity effects in two-dimensional van der Waals heterostructures are an efficient way to modify intrinsic electronic properties[1]. In particular, proximity exchange offers the possibility of inducing magnetic properties in nominally nonmagnetic materials. Furthermore, this induced synthetic Zeeman splting exhibits strong signatures in the optical spectra. Combining ab initio calculations with tight-binding modeling and the effective Bethe-Salpeter equation for excitons, we investigate the proximity exchange in TMDC/ferromagnet systems: (i) (Mo,W)Se2 on the ultrathin van der Waals ferromagnet CrI3[2] and (ii) (Mo,W)S2/hBN on ferromagnets Co and Ni[3]. Since stacking different 2D materials requires adjusting the lattice parameters to obtain commensurate supercells, we also discuss the impact of biaxial strain in monolayer TMDCs[4]. We show the evolution of different optical transitions and the role of excitonic effects in the direct transitions. [1] Zutic et al., Mater. Today 22, 85 (2019). [2] Zollner, Faria Junior, Fabian, PRB 100, 085128 (2019). [3] Zollner, Faria Junior, Fabian, arXiv:1910.13223 (2019). [4] Zollner, Faria Junior, Fabian, PRB 100, 195126 (2019). Supported by: Alexander von Humboldt Foundation, Capes, DPG SFB 1277.

DS 22.11 Wed 12:30 POT 81

Decreasing Activation Energies with Thickness of Thin $HfTe_5$ layers — •Christopher Belke[1], Sonja Locmelis[2], Lars Thole[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

Hafnium pentatelluride ($HfTe_5$) is a layered two dimensional material from the class of Transition Metal Penta Chalcogenide with the chemical formula MX_5, where M is a transition metal and X a chalcogenide [1]. $HfTe_5$ shows a resistivity anomaly and is expected to be a topological insulator [2] with a bulk band gap of about 22 meV [3]. In addition, theory predicts that a single layer should show a band gap of about 400 meV and should be a quantum spin hall insulator [1].

We present that the electronic properties of $HfTe_5$ drastically change with decreasing thickness. We prepared samples with different thicknesses under 100 nm and made temperature dependent measurements to determine the activation energy in an Arrhenius plot. We found that the band gap increases with decreasing thickness. Conductivity measurements also show an anomaly due to a mobility change at around 120 K.

[1] H. Weng et al., Phys. Rev. X 4, 011002 (2014)
[2] S. Liu et al., APL Materials 6, 121111 (2018)
[3] H. Wang et al., Phys. Rev. B 93, 165127 (2016)

DS 22.12 Wed 12:45 POT 81

Tailoring of electronic and magnetic properties of hematene: a computational study — •Yidan Wei, Mahdi Ghorbani, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Exfoliation of non van der Waals materials has established new class of two dimensional materials, such as hematene btained from hematite. In order to exploit and design potential applications, understanding the electronic and magnetic properties is crucial. Using density functional theory calculations, the atomic structures, electronic and magnetic properties of hematene are systematically investigated. Bare hematene in the ferromagnetic states is less stable than that in the anti ferromagnetic states, and it has a direct band gap. The stability, electronic and magnetic properties of hematene can change significantly with different terminations. Hematene covered with OH is a semiconductor with surface states removed, while hematene covered with H changes from semiconductor to half metal. Further, changes in the electronic characteristics are possible under with mechanical deformation. Applying strain causes significant changes in the electronic properties of hematene. In case of non-terminated hematene, both compressive and tensile strain can result in a reduction of the band gap in the anti-ferromagnetic state under biaxial and uniaxial deformation, and the band gap increases in case of OH terminated hematene. The band gap also increases under tensile strain in the ferromagnetic states. The deformation can lead to the enhancement of polarization.