DS 44: Physics and Application of Emergent 2D-semiconductors and their Heterostructures I (Joint session of DS and HL, organized by DS)

Time: Thursday 11:15–13:15 Location: H8

DS 44.1 Thu 11:15 H8

Defects in two-dimensional materials: their production under irradiation, evolution and properties from first-principles calculations — •Arkady Krasheninnikov — Helmholtz Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Germany — Department of Applied Physics, Aalto University, Finland

Following isolation of a single sheet of graphene, many other 2D systems such as hexagonal BN and transition metal dichalcogenides (TMDs) were manufactured. Among them, TMD sheets have received particular attention, as these materials exhibit intriguing. Moreover, the properties can further be tuned by introduction of defects and impurities. In my talk, I will present the results [1] of our first-principles theoretical studies of defects (native and irradiation-induced) in inorganic 2D systems obtained in collaboration with several experimental groups. I will further discuss defect- and impurity-mediated engineering of the electronic structure of 2D materials.

[1] Nature Comm. 6 (2015) 6736; ACS Nano 9 (2015) 3274; ACS Nano (2015) DOI: 10.1021/acsnano.5b04851; Phys. Rev. B 91 (2015) 125304; Adv. Mater. 26 (2014) 2857; Phys. Rev. X 4 (2014) 031044; see http://physics.aalto.fi/~ark/publist.html for complete list of publications.

DS 44.2 Thu 11:30 H8

Phonon induced line broadening and population of the dark exciton in a deeply trapped localized emitter in monolayer WSe2 — •Yu-Ming He[1,3], Chao-Yang Lu[3], Jian-Wei Pan[3], Sven Höfling[1,2,3], and Chrisitian Schneider[1] — [1]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS,United Kingdom — [3]Hefei National Laboratory for Physical Sciences at the Microscale and Department of Modern Physics, & CAS Center for Excellence and Synergetic Innovation Center in Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

We study locally trapped single excitons in a mechanically exfoliated WSe2 monolayer semiconductor with respect to their temperature stability, spectral diffusion and decay dynamics. We identify strong signatures of phonon induced spectral broadening in these emitters for elevated temperatures accompanied by temperature induced luminescence quenching. A direct correlation between the drop in intensity at higher temperatures with the phonon induced population of dark states in WSe2 is established.

DS 44.3 Thu 11:45 H8

Gate voltage dependence of the electron mobility in monolayer $MoS_2 - LiNbO_3$ field effect transistors — •Wladislaw Michailow[1], Edwin Preciado[2], Florian Schülein[1], Benjamin Möller[1], Ariana Nguyen[2], David Barroso[2], Miguel Isarraraz[2], Gretel von Son[2], I-Hsi Lu[2], Velveth Klee[2], John Mann[2], Andreas Hörner[1], Achim Wixforth[1], Ludwig Bartels[2], and Hubert Krenner[1] — [1]Insitut für Physik, Universität Augsburg, Germany — [2]University of California, Riverside, USA

In field effect transistors (FETs) based on novel two-dimensional semiconductor materials, detailed knowledge of the density and the mobility of charge carriers in the conducting channel is of paramount importance. In the most common approach the field effect mobility and charge carrier density are determined by a simple parallel-plate capacitor model. In this model the carrier mobility is assumed to be independent of the gate potential. Here we report on investigations of monolayer $MoS_2 - LiNbO_3$ FETs [1] in which we determined the source-drain current and the capacitance as function of gate voltage. We analyze both using a theoretical model of a two-dimensional free electron gas. This analysis allows us to derive both the charge carrier density and the mobility over the full $\pm 40\,V$ range of gate voltage. Using our advanced analysis we show that for our structure the established parallel-plate capacitor model is oversimplified and overestimates the carrier mobility by a factor of $\gtrsim 4$.

[1] E. Preciado et al., Nat. Commun. **6**, 8593 (2015).

DS 44.4 Thu 12:00 H8

Resistivity switching in chalcogenide based interfacial phase change materials — •Nicki F. Hinsche and Kristian S. Thygesen — Center for Atomic-scale Materials Design, Technical University of Denmark, 2830 Kgs. Lyngby, Denmark

Chalcogenide based phase change materials (PCM) are emerging candidates for next generation non-volatile, ultra-fast memories. In contrast to conventional amorphous-crystal phase transition driven PCM, e.g. $Ge_2Sb_2Te_5$, recently a new type of PCM device named *interfacial phase change memory* (iPCM) was proposed [1]. Here the electrical pulse induced movement of the atoms is limited to the interface, therefore substantially reducing the switching energies and allowing for shorter switching times.

By means of DFT electronic-structure [2] and Boltzmann transport calculations [3], we discuss for an iPCM GeTe-Sb_2Te_3 heterostructure the electrical resistivity change caused by the structural switching at the interface. With a close relation of the material system to the family of topological insulators, ferroelectrics [4] and thermoelectrics, the possibility of a ferroelectric controllable topological phase transition and the ultra-fast modification of the thermoelectric properties, applicable for fast thermal switches, will be analysed additionally.

[1] R. E. Simpson *et al.*, Nature Nanotechnology **6** 8501(2011); [2] J. Enkovaara *et al.*, J. Phys.: Condens. Matter **22** 253202 (2010); [3] N. F. Hinsche *et al.*, ACS Nano **9** 4406 (2015) [4] A. V. Kolobov *et al.*, APL Mater. **2** 066101 (2014)

DS 44.5 Thu 12:15 H8

Electrical properties of CVD Molybdenum disulfide — •Wajid Awan[1], Tommy Schönherr[1], Artur Erbe[1], Stefan Facsko[1], and Xinliang Feng[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Technische Universität Dresden

Two dimensional materials are attractive for the use in next-generation nanoelectronic devices as compared to one dimensional material because it is relatively easy to fabricate complex structures from them. Recently the layered 2D semiconducting Transition metal dichalcogenides came into the picture and got a place in a wide range of novel applications as well as in basic research. Strikingly, MoS_2 receives significant attention since it undergoes transition from indirect bandgap (bulk form) to a direct bandgap (1.2eV) semiconductor if thinned out to a single atomic layer. The bandgap is an essential property for tunable 2-D nanodevices. We performed electrical transport measurements at room temperature for CVD grown MoS_2 on SiO_2/Si substrate. Standard Electron beam lithography (EBL) was used to pattern Gold (Au) metal contacts on MoS_2 flakes. For the purpose of sample characterization, we performed the Atomic Force Microscopy (AFM) and Raman Spectroscopy techniques, respectively, which confirm that the thickness of the CVD grown MoS_2 triangular flakes corresponds to single layers. Low temperature characterization of the electrical properties of the layers elucidates the exact mechanisms of charge transport in the 2d-layers. This knowledge will be used to modify the electrical properties in a controlled way, for example by ion irradiation.

DS 44.6 Thu 12:30 H8

Nonlinear Optics in a Rydberg-Excited Semiconductor Cavity — •Valentin Walther, Robert Johne, and Thomas Pohl — Max Planck Institute for the Physics of Complex Systems, Dresden

Recent experiments have demonstrated excitons with extraordinarily large binding energies in some two-dimensional semiconductors (TMDCs), whose Rydberg states give rise to giant interactions and, therefore, hold great promise for optical utility.

We evaluate the optical response under conditions of electromagnetically induced transparency (EIT), accounting for the full excited level structure and numerous decoherence mechanisms in a semiconductor. Strong exciton-exciton interactions result in enormous effective photon-photon potentials. Using experimental parameters, we show that the photonic nonlinearity exceeds that of traditional semiconductors by several orders of magnitude and we assess the material properties required for coherent optical applications.

Further, we investigate interesting optical effects in the transverse mode structure of a driven-dissipative cavity arising from the unusually large nonlinearity.

DS 44.7 Thu 12:45 H8

Thermal expansion and transport in van-der-Waals solids from first-principles — •Daniel Lindroth, Per Hyldgaard, and Paul Erhart — Chalmers University of Technology, Gothenburg, Sweden

We have performed first-principles calculations for lattice thermal expansion and transport in the bulk of the transition metal dichalcogenides (TMDCs) MoS2, MoSe2, MoTe2, WS2, WSe2 and WTe2 using density functional theory (DFT) and the semi-classical phonon Boltzmann transport equation (BTE) within the relaxation time approximation (RTA).

Proper modeling of the lattice thermal conductivity is important for an accurate prediction of the thermoelectric figure of merit and better understanding of potentially high performing novel materials such as van der Waals heterostructures based on TMDCs. To this end, we have conducted a thorough investigation of the mentioned TMDCs based on DFT calculations using a recently published van der Waals density functional (vdW-DF-cx) in conjunction with anharmonic modeling of phonon lifetimes using third order interatomic force constants that allows for solutions to the BTE within the RTA as implemented in the phono3py code. We found that our calculations agrees with theoretical expectations as well as with experimental data where available. The methods used thus provide a promising framework for further investigation of more complex systems with potentially novel thermal properties.

DS 44.8 Thu 13:00 H8

Enabling a new class of electronic devices using self-aligned nanodomain boundaries to open a charge transport gap in trilayer graphene — •Victor Aristov[1,2,3], Olga Molodtsova[1,4], Sergey Babenkov[1], Tsung-Wei Huang[5], Askar Syrlybekov[6], Mourad Abid[7], Dmitry Marchenko[8], Jaime Sánchez-Barriga[8], Partha Sarathi Mandal[8], Andrei Varykhalov[8], Yuran Niu[9], Barry Murphy[6], Sergey Krasnikov[6], Olaf Lübben[6], Alexander Chaika[2,6], and Han-Chun Wu[6] — [1]DESY, Hamburg, Germany — [2]ISSP RAS, Chernogolovka, Russia — [3]TU Bergakademie, Freiberg, Germany — [4]ITMO, Saint Petersburg, Russia — [5]National Taiwan University, Taipei, Taiwan — [6]Trinity College, Dublin, Ireland — [7]King Saud University, Riyadh, Saudi Arabia — [8]BESSY, Berlin, Germany — [9]Max-lab, Lund, Sweden

Trilayer graphene reveals unique electronic properties interesting for fundamental science and technological applications. The ability to achieve a high on-off current ratio is the central question in this field. We propose a simple method to achieve a current with high on-off ratio by opening a transport gap in trilayer graphene with self-aligned periodic nanodomain boundaries (NBs). Our low temperature transport measurements clearly demonstrate that the self-aligned periodic NBs induce a huge charge transport gap, more than 1.3 eV at 10 K. As a result of our study the feasibility of creating new electronic nanostructures with high on-off current ratios using graphene on cubic-SiC/Si wafers was shown. This work was supported by the RAS, RFBR grants No 140200949 and 140201234, by SPP 1459 of DFG.