DS 22: Two-dimensional materials III (jointly with HL/TT)

Time: Tuesday 9:30–13:15 Location: POT 51

DS 22.1 Tue 9:30 POT 51

Optical properties of organic/inorganic and all-inorganic lead halide perovskite nanoplatelets — •Jasmina A. Sichert[1,2], Yu Tong[1,2], Verena A. Hintermayr[1,2], Alexander F. Richter[1,2], Bernhard Bohn[1,2], Lakshminarayana Polavarapu[1,2], Carlos Cardenas-Daw[1,2], Alexander S. Urban[1,2], and Jochen Feldmann[1,2] — [1]Chair for Photonics and Optoelectronics, Department of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität (LMU), Amalienstaße 54, 80799 Munich, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 Munich Germany

In recent years, organic/inorganic and all-inorganic lead halide perovskite have shown great potential for photovoltaics as well as for light-emitting applications. We have successfully synthesized two-dimensional methylammonium and cesium lead halide perovskite nanoplatelets of varying thickness down to one monolayer.[1,2] With decrease in crystal thickness we observed quantum-size effects and an increase in the exciton binding energy. In the extreme case of a perovskite sheet only a single unit cell thick, the screening of the exciton decreases significantly, resulting in a huge exciton binding energy of several hundred meV in the thin nanoplatelets. We conducted time-resolved photoluminescence spectroscopy to further investigate the effect of the crystal thickness on the optical properties of the nanoplatelets.

[1] Sichert et al., Nano Lett. 15, 6521-6527 (2015)
[2] Tong et al., Angew. Chem. 55, 13887-13892 (2016)

DS 22.2 Tue 9:45 POT 51

Band-gap and exciton binding-energy renormalizations due to excited carriers in monolayer TMDs — •Daniel Erben[1], Christopher Gies[1], Malte Rösner[1,2], Alexander Steinhoff[1], Matthias Florian[1], Michael Lorke[1], Tim Wehling[1,2], and Frank Jahnke[1] — [1]Insitute for Theoretical Physics, University of Bremen, Germany — [2]Bremen Center for Computational Materials Science, University of Bremen, Germany

Coulomb interaction between charge carriers in atomically thin layers of transition-metal dichalcogenides (TMDs) has been shown to be exceptionally large due to the weak screening in the thin layer itself. It causes strong renormalization effects which change the electronic properties and the optical response of the material.

We investigate excited-state optical properties of the typical monolayer TMDs MoS_2, $MoSe_2$, WS_2 and WSe_2 by solving the semiconductor Bloch equations on the full Brillouin zone using the SXCH-approximation for the Coulomb interaction. Excitonic resonances shift in absolute value and relative to each other with increasing carrier density. This effect is a result of a band-gap reduction due to many-particle renormalizations and a reduction of the binding energy due to screening of the Coulomb interaction and Pauli blocking, which we analyse and compare in detail for MoS_2, $MoSe_2$, WS_2 and WSe_2. Our calculations predict a transition from a direct to an indirect band-gap in molybdenum and tungsten disulfides in the presence of highly excited carriers. The selenides stay indirect for different excitations.

DS 22.3 Tue 10:00 POT 51

Phase separation and composition fluctuation effects on electronic and optical properties of $(BN)_{1-x}(C_2)_x$ 2D alloy — •Ivan Guilhon[1], Lara K Teles[1], Marcelo Marques[1], and Friedhelm Bechstedt[2] — [1]Grupo de Materiais Semicondutores e Nanotecnologia, Instituto Tecnológico de Aeronáutica, DCTA, 12228-900 São José dos Campos, Brazil — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, D-07743 Jena, Germany

$(BN)_{1-x}(C_2)_x$ alloys are promising materials for band gap engineering in two-dimensional electronics. Despite the importance of microstructural features, such as phase separation and composition fluctuation. The current theoretical studies of such monolayer alloys are often restricted to investigate "guessed" nonrandom structures.

Using DFT calculations combined with a statistical approach to account for disorder effects, we study the properties of these 2D alloys as a function of their average composition. A complete scenario of how thermodynamic conditions affect the distribution of atoms is provided. The solubility limits and critical temperature are studied by constructing a T-x phase diagram.

In this context, we calculate the energy gap as a function of the composition and optical absorbance spectra are predicted for different compositions. Our predictions are compared with the experimental findings. We reproduce the experimentally found absorption spectra with a two-peak pattern for intermediate carbon concentrations and identify them with phase-segregated instead of homogeneous alloys.

DS 22.4 Tue 10:15 POT 51

Electron-phonon interaction in transition metal dichalcogenides — •Nicki F. Hinsche[1], Arlette Sohanfo Ngankeu[2], Sanjoy Mahatha[2], Marco Bianchi[2], Charlotte Sanders[2], Philip Hofmann[2], and Kristian S. Thygesen[1] — [1]Center for Atomic-scale Materials Design, Technical University of Denmark, 2830 Kgs. Lyngby, Denmark — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark

Atomically thin layers of Transition Metal Dichalcogenides (TMD) attract remarkable interest due to their extraordinary electronic and optical properties and are often quoted as semiconductor analogues of graphene. Possessing direct band gaps in the visible frequency range and exhibiting high electronic mobilities at room temperature, TMD's are emerging candidates for next generation electronic and optoelectronic applications [1]. By means of DFT electronic-structure and Boltzmann transport calculations [2], we discuss the impact of microscopic electron-phonon interaction onto the renormalization of the electronic structure and the phonon-limited electronic transport properties for two prototypical TMD's: TaS_2 and WS_2. Our analysis and conclusions will be drawn closely to recent experimental findings [3].

[1] F. A. Rasmussen and K. S. Thygesen. Journ. of Phys. Chem. C **13** 169 (2015) [2] N. F. Hinsche *et al.*, ACS Nano **9** 4406 (2015) [3] C. E. Sanders *et al.*, Physical Rev. B. **94** 081404 (2016)

DS 22.5 Tue 10:30 POT 51

Spin Degenerate Regimes for Single Two-Dimensional Quantum Dots on Transition Metal Dichalcogenide Monolayers — •Matthew Brooks and Guido Burkard — Department of Physics, University of Konstanz, D-78464, Germany

Strong spin orbit coupling in transition metal dichalcogenides (TMDCs) monolayers results in spin resolvable band structures about the K (K') valleys such that the eigenbasis of a 2D quantum dot (QD) on a TMDC monolayer in zero field is described by the Kramers pairs $|+\rangle = |K' \uparrow\rangle, |K \downarrow\rangle$ and $|-\rangle = |K \uparrow\rangle, |K' \downarrow\rangle$. This coupling limits the usefulness of single TMDC QDs as qubits due to the inherent difficulty of generating superposition states of the valley degree of freedom. Possible regimes of spin degenerate states overcoming the spin orbit coupling in monolayer TMDC QDs are investigated in both zero field, where the spin and valley degrees of freedom become fourfold degenerate, and in some magnetic field, localised to the K' valley. Such regimes are shown to be achieved in MoS_2, where the spin orbit coupling is sufficiently low that the spin resolved conduction bands intersect at points about the K (K') valleys and as such may be exploited by selecting suitable critical dot radii.

DS 22.6 Tue 10:45 POT 51

Electron Spin Relaxation in a Transition-Metal Dichalcogenide Quantum Dot — •Alexander Pearce and Guido Burkard — University of Konstanz, Konstanz, Germany

We study the relaxation of a single electron spin in a circular quantum dot in a transition-metal dichalcogenide monolayer defined by electrostatic gating. Transition-metal dichalcogenides provide an interesting and promising arena for quantum dot nano-structures due to combination of spin-valley physics and strong spin-orbit coupling. First we will discuss which bound state solutions in different B-field regimes can be used as the basis for qubits, at low B-fields combined spin-valley Kramers qubits and at large B-fields spin qubits. Then we will discuss the relaxation of a single electron spin mediated by electron-phonon interaction via various different relaxation channels. Rashba spin-orbit admixture mechanisms allow for relaxation by in-plane phonons arising either from the deformation potential or by piezoelectric coupling, additionally direct spin-phonon mechanisms involving out-of-plane phonons allow for relaxation. We find that the relaxation rates

scale as $\propto B^4$ and $\propto B^2$ for in-plane phonons coupling via deformation potential and piezoelectric coupling respectively, while relaxation due to the direct spin-phonon coupling scales as $\propto B^2$. In the low B-field regime we also discuss the role of impurity mediated spin relaxation which will arise in disordered quantum dots.

Coffee Break

Invited Talk DS 22.7 Tue 11:30 POT 51

Influence of dark states on excitonic spectra of transition metal dichalcogenides — •Malte Selig[1,2], Dominik Christiansen[1], Gunnar Berghäuser[1,2], Ermin Malic[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

In monolayers of transition metal dichalcogenides, excitonic effects play a significant role: Besides bright excitons, dark exciton states are formed by electrons and holes with opposite spin or constitute excitons with non-vanishing center of mass momentum well above the lightcone. Evaluating the excitonic states it turns out, that in tungsten based materials some of these dark states are energetically located below the optical accessible ones. Here, we develope excitonic Bloch equations for excitonic polarizations and densities under the influence exciton phonon interaction, adressing the strong impact of low lying dark states. We investigate the dephasing of the excitonic polarization through exciton phonon scattering [1] and the phonon mediated formation and thermalization of exciton densities. It turns out that coupling to low lying dark states is crucial for luminescence yield and lifetime. The presented results can explain several recent experimental results.

[1] M. Selig et al.,Nature Commun. 7,13279 (2016)

DS 22.8 Tue 12:00 POT 51

Transport measurements in graphene-WSe_2 heterostructures — •Tobias Völkl[1], Tobias Rockinger[1], Martin Drienovsky[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Universität Regensburg, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

Bringing graphene into proximity to WSe_2 was proposed as a way to induce a high spin orbit coupling strength in graphene, while maintaining the high intrinsic mobility of graphene. We therefore investigated the transport properties of graphene-WSe_2 heterostructures.

Placing graphene onto a WSe_2-flake resulted in mobilities around 10000 cm^2/Vs of graphene. Further a weak antilocalization behavior was observed, which indicates a high spin orbit coupling strength induced by the WSe_2.

Higher mobilities around 100000 cm^2/Vs were achieved by encapsulation of graphene between WSe_2 and hBN. In these samples no weak antilocalization behavior could be observed. We attribute this to a transition from diffusive to the quasiballistic regime. Also a feature dependent on the sample width arises in the low magnetic field range. We attribute this to a magneto size effect which further indicates quasiballistic behavior.

DS 22.9 Tue 12:15 POT 51

Electrical behavior of the oxidation of atomically thin $HfSe_2$ under ambient conditions — •Christopher Belke, Hennrik Schmidt, Benedikt Brechtken, Johannes C. Rode, Dmitri Smirnov, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover

12 years after the discovery of graphene [1], two-dimensional materials are of rising importance in the research and development section. An example for those layered materials are TransitionMetalDichalcogenide (TMD) with the chemical formula MX_2 , where M is a transition metal and X a chalcogenide [2]. Some materials are very fragile in ambient conditions. One of them is the n-type semiconductor hafnium diselenide ($HfSe_2$) [3]. During the fabrication the samples were prepared under nitrogen atmosphere or were covered with PMMA. An increasing resistance was measured while the sample was oxidized under ambient conditions, as well as a change of the electric field effect was observed.

[1] A. K. Geim et al., Nature Materials, **6**, 183 (2007)
[2] A. K. Geim, and I. V. Grigorieva, Nature **499**, 419 (2013)
[3] M. Kang et al. APL **106**, 143108 (2015)

DS 22.10 Tue 12:30 POT 51

ab initio **study of the transport properties in bulk and monolayer MX_3 (M = Ti, Zr, Hf and X = S, Se) compounds.** — •Yasir Saeed — Qatar Environment and Energy Research Institute (QEERI), Hamad Bin Khalifa University (HBKU), Qatar Foundation, P.O. Box 5825, Doha, Qatar

Two dimensional (2D) materials are best candidates for thermoelectric application due to their low thermal conductivity which is key property to achieve high efficiency for their usage in the filed of energy harvesting. Owing to that, here we present a study on electronic as well as thermal transport of bulk and monolayer MX_3 compounds (M = Ti, Zr, and Hf and X = S and Se) are investigated by by density functional theory and semi-classical Boltzmann theory. The bandgap amounts to rather similar value for bulk and monolayer, only the shape of band near Fermi level changes slightly, which results in a modified effective mass. We found that monolayer MX_3 compounds are good TE materials than bulk. Also *p*-type monolayer TiS_3 has twice large PF at 600 K than its room temperature value. However, monolayer $Zr/HfSe_3$ compounds showing promising behavior as a *n*-type TE materials at elevated high temperature of 600 K. In-plane tensile strain is also possible to tune the bandgap to increase S and disorder the monolayer lattice to minimize κ, therefore turns out to be a highly efficient approach for creating high performance TE materials.

DS 22.11 Tue 12:45 POT 51

Nonlinear Hall voltage from magnetic hot-spots — •Karina A. Guerrero Becerra, Andrea Tomadin, Andrea Toma, Remo Proietti Zaccaria, Francesco De Angelis, and Marco Polini — Istituto Italiano di Tecnologia, via Morego 30, I-16163 Genova, Italy

Electromagnetic simulations have recently shown that specifically designed plasmonic nanostructures are able to enhance and localize an oscillating magnetic field within a micro-meter area. These magnetic hot-spots, generated by forcing the plasmonic resonances of planar nanostructures to generate displacement currents of coil-type shape, have been shown to operate in the NIR [A. Nazir, *et. al.* Nano. Lett., 14, 3166-3171 (2014)] and in the MIR [S. Panaro, *et. al.* Nano. Lett., 15, 6128-6134 (2015)] frequency regions. Operating frequencies can be extended towards the THz regime. Here we propose that magnetic hot-spots might be probed through transport measurements by exploiting the response of the 2D electron gas (2DEG) hosted in a graphene bar, placed within the hot-spot area. We study the response of the 2DEG, being subject to the oscillating in-plane electric field of the radiation driving the coil-type resonance, and to the localized magnetic field induced by it. We found that the response of the graphene 2DEG drives a rectification effect giving rise to a measurable Hall-like dc voltage, being sensitive to the operational frequency of the hot-spot. We discuss the conditions under which the predicted dc voltage is experimentally accessible, within the range of frequencies from THz to MIR. We show that the electric and magnetic fields within the hot-spot launch graphene plasma waves.

DS 22.12 Tue 13:00 POT 51

Exchange Interaction for Quantum Dots in TMDCs — •Alessandro David, Andor Kormanyos, and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We study the properties of double quantum dots in Transition Metal Dichalcogenides (TMDCs) where trapped electrons comprise not only the usual spin and valley degrees of freedom, but also a spin-orbit splitting in the spectrum. The spin-orbit coupling splits the four-fold spin and valley degeneracy into two Kramers pairs with correlated spin and valley states. We consider two different situations where the spin-orbit splitting is either much larger or comparable to the tunneling. Our aim is to use such systems filled with only two electrons for quantum information processing. In the case of large spin-orbit splitting, it turns out that there is a fourfold degenerate ground state (well separated from higher states) where, with a simple redefinition of Pauli matrices, we can obtain a CNOT gate in the same way it was obtained in the quantum computer proposed by Loss and DiVincenzo. In the case of small spin-orbit splitting, we have to consider a 16 dimensional subspace, but it is still possible to obtain a unitary evolution operator, that also depends on the value of spin-orbit splitting.