O 10: Two-dimensional Materials

Time: Monday 9:30–13:00 Location: H16

O 10.1 Mon 9:30 H16

Boundary conditions for transition-metal dichalcogenide monolayers in the continuum model — •Csaba Géza Péterfalvi, Andor Kormányos, and Guido Burkard — Department of Physics, University of Konstanz, D-78464 Konstanz, Germany

We derive the boundary conditions for MoS_2 and similar transition-metal dichalcogenide honeycomb (2H polytype) monolayers with the same type of $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian within the continuum model around the K points. [1] In an effective 2-band description, the electron-hole symmetry breaking quadratic terms are also taken into account. We model the effect of the edges with a linear edge constraint method that has been applied previously to graphene. Focusing mainly on zigzag edges, we find that different reconstruction geometries with different edge-atoms can generally be described with one scalar parameter varying between 0 and 2π. We analyze the edge states and their dispersion relation in MoS_2 in particular, and we find good agreement with the results of previous density functional theory calculations for various edge types.

[1] Cs. G. Péterfalvi, A. Kormányos, G. Burkard, arXiv:1509.00184 (2015).

O 10.2 Mon 9:45 H16

High Q-factor in WSe2 Nano-electromechanical resonator — •Antoine Reserbat-Plantey[1], Nicolas Morell[1], Ioannis Tsioutsios[1], Kevin Schädler[1], François Dubin[2], Frank Koppens[1], and Adrian Bachtold[1] — [1]ICFO, The Insitutue for Photonic Sciences, Barcelona, ES — [2]INSP, Université Paris 6, Paris, FR

Atomically thin nano-electromechanical systems (2D-NEMS) combine extremely low mass resonators having resonant frequencies in the MHz-GHz range, wide tunability, low damping and exotic non-linearities. Atomically thin 2D semi-conductors such as transition metal dichalcogenides (TMD) have extremely rich optical properties (direct band gap, spin valley, embedded quantum emitters), which are intrinsically linked to their low dimensionality. Optical and electronic properties of WSe2, an emblematic TMD, have been intensively studied while there is no extensive nanomechanical investigation of this system. Here we show a new generation of semiconductor 2D-NEMS made of monolayer of WSe2. We record mechanical and photoluminescence spectra of WSe2 nanoresonators down to cryogenic temperatures. We measure mechanical quality factor Q>47000 at T=3.5 K, which is the highest value reported so far for 2D-NEMS in this temperature range. Combining ultra-low dissipation resonators with the very rich optical properties of TMD, paves the way for novel type of optomechanical experiments with 2D materials.

O 10.3 Mon 10:00 H16

Landau levels and Shubnikov-de Haas oscillations in monolayer transition metal dichalcogenide semiconductors — •Andor Kormányos[1], Péter Rakyta[2], and Guido Burkard[1] — [1]Physics Department, University of Konstanz — [2]Department of Theoretical Physics, Budapest University of Technology and Economics

We study the Landau level (LL) spectrum using a multi-band $\mathbf{k}\cdot\mathbf{p}$ theory in monolayer transition metal dichalcogenide semiconductors [1]. We find that in a wide magnetic field range the LL can be characterized by a harmonic oscillator spectrum and a linear-in-magnetic field term which describes the valley degeneracy breaking. The effect of the non-parabolicity of the band-dispersion on the LL spectrum is also discussed. Motivated by recent magnetotransport experiments, we use the self-consistent Born approximation and the Kubo formalism to calculate the Shubnikov-de Haas oscillations of the longitudinal conductivity. We investigate how the doping level, the spin-splitting of the bands and the broken valley degeneracy of the LLs affect the magnetoconductance oscillations. We consider monolayer MoS_2 and WSe_2 as concrete examples and compare the results of numerical calculations and an analytical formula which is valid in the semiclassical regime. Finally, we briefly analyze the recent experimental results [Cui et al., Nat. Nanotechnol. **10**, 534 (2015)] using the theoretical approach we have developed.

[1] New J. Phys. **17**, 103006 (2015).

O 10.4 Mon 10:15 H16

Second-harmonic generation in MoS2 monolayers coupled to resonant nanoantennas — •Franz Johannes Friedrich Löchner[1], Stefan Fasold[1], Antony George[2], Paul Douglas Harrison[1], Christoph Menzel[1], Andrey Turchanin[2], Isabelle Staude[1], Falk Eilenberger[3], Frank Setzpfandt[1], and Thomas Pertsch[1] — [1]Institute of Applied Physics, Abbe Center of Photonics , Friedrich-Schiller-Universität Jena, 07743 Jena, Germany — [2]Institute of Physical Chemistry, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany — [3]Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

Two-dimensional monolayers of transition metal dichalcogenides (TMDs), a new class of direct band-gap semiconductors, recently have attracted a lot of attention due to their pronounced excitonic emission lines and strong second-order nonlinearity.

Coupling TMDs to resonant nanoantennas allows to further enhance these effects by concentrating the exciting optical field into a small volume. Such enhancement has been shown for excitonic emission using plasmonic nanoantennas. However, nonlinear optical effects in TMD-nanoantenna systems have not been studied yet.

In our contribution, we report on experimental investigations of second-harmonic generation in molybdenum disulfide (MoS2) monolayers coupled to nanoantennas, resonant at the exciting fundamental-harmonic wavelength. Polarization resolved measurements show the profound impact which the presence of the nanoantenna has on the second-harmonic radiation generated by the MoS2-monolayer.

O 10.5 Mon 10:30 H16

Electrochemical growth and characterization of molybdenum sulfide layers for thin film transistors — •Talha Nisar, Torsten Balster, and Veit Wagner — Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany

Molybdenum disulfide has attracted considerable interest for its great potential in the field of nanoelectronics due to its semiconducting and 2D nature. It has been successfully deposited by the Scotch tape method resulting in high-mobility transistors with an area of a few square microns. The state-of-the-art method for the growth of crystalline molybdenum disulfide single and multilayers is chemical vapor deposition.

In our study we use electrochemical deposition as an alternative approach to grow large area molybdenum sulfide layers. For this purpose, ammonium tetrathiomolybdate (ATTM) has been used as precursor material for the electrodeposition in cathodic regime with respect to Ag/AgCl reference electrode. The obtained layers are amorphous as could be confirmed by Raman measurements. In addition, in the UV-VIS spectra of the MoS_x (x=2..3) layer a transition at 2.4 eV is visible, which could be related to oxygen contamination. Further annealing steps in an Ar/H_2 atmosphere with an additional sulfur source at temperatures above 600°C are necessary to remove the oxygen and to convert the layer into crystalline MoS_2. The converted layer has to be transferred onto SiO_2/Si substrates for thin film transistor applications.

30 min. Coffee Break

Invited Talk O 10.6 Mon 11:15 H16

Epitaxial paradigms of van der Waals bonded chalcogenide materials — •Raffaella Calarco — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

In recent years it has become clear that materials with covalent bonding in only two dimensions (2D) have attractive properties for devices. The bonding in the third dimension, which is between individual layers, occurs by van der Waals (vdW) forces, which are weaker if compared to the covalent bonding. Materials used in conventional devices are instead characterized by covalent bonding in three dimensions (3D). In the present contribution, I shed some light on understanding the mechanisms that determine the interface structure between 2D and 3D or 2D materials. To study possible options for altering the bonding configurations of the 2D-3D interface GeTe-Sb2Te3 layers are deposited by molecular beam epitaxy on top of five different surface reconstructions-passivation of the Si(111). The 2D-2D interface is best studied using graphene as a substrate. Finally, I address the most crucial issue: The realization of vdW epitaxy in Sb2Te3-GeTe superlattices. Such superlattices, if compared to their alloy counterpart, show impressive

performances highly attractive for future non-volatile memory applications.

O 10.7 Mon 11:45 H16

Transparent Conducting Materials: Insights from High-Throughput — •Pino D'Amico[1,2], Alice Ruini[1,2], Alessandra Catellani[2], Arrigo Calzolari[2], Marco Fornari[3,5], and Marco B. Nardelli[4,5] — [1]FIM-UNIMORE, Modena, Italy — [2]CNR-NANO S3, Modena, Italy — [3]Central Michigan Univ., Mt. Pleasant, USA — [4]Univ. of North Texas, Denton, USA — [5]Duke Univ., Durham, USA

Good electrical conductivity and optical transparency in the visible domain are the physical properties required in order to have Transparent Conducting Material (TCM). Various semiconductors becomes TCM when doped and up to now their discovery has followed an a-posteriori path: take a material and investigate its physical properties in order to see if it is a good TCM. Thanks to the large amount of data available in the AFLOWLIB repository[1], we use instead an inverse-design approach in order to search for new possible TCMs: starting from the paradigmatic case of ZnO[2] we have identified the physical descriptors representing a TCM and extracted from the database a list of materials having the required characteristics using highthroughput techniques. We investigated doped structures of resulting materials inserting substitutional elements in a systematic way with a given concentration. We will present an accurate study of both conductivity and optical properties of the doped structures obtained by means of a newly developed numerical tool based on Boltzmann theory and dielectric function calculations[3] and reliyng on an efficient ab-initio tight-binding representation of the lattice structures[4]. [1]www.aflowlib.org; [2]ACS Photonics 1, 703 (2014); [3]preprint(2015); [4]arXiv:1509.02558 (2015).

O 10.8 Mon 12:00 H16

Investigating the Potential of TMD Monolayers as Photodetectors — •Maja Feierabend[1], Gunnar Berghäuser[2], and Ermin Malic[2] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

Transition metal dichalcogenides (TMDs) are promising materials for technological application in the area of optoelectronics. Due to the direct band gap and the extraordinarily strong Coulomb interaction, TMDs exhibit efficient light-matter coupling and tightly bound excitons [1]. As atomically thin materials, they are very sensitive to changes in the surrounding environment. This motivates a functionalisation approach, where external molecules are non-covalently attached to the material surface to control its optical properties.

Here, we theoretically investigate functionalized TMDs based on the density matrix formalism combined with tight-binding wave functions. Considering exemplary spiropyran molecules exhibiting a strong dipole moment, we predict pronounced spectral red-shifts and the appearance of an additional side-peak in the absorption spectrum of functionalized TMDs. Interestingly, we also observe a further peak splitting due to the intervalley coupling between the high-symmetry K/K' points. The predicted pronounced changes in optical spectra of TMDs show their potential for technological application in photodetectors.

[1] G. Berghäuser and E. Malic, PRB 89, 125309 (2014)

O 10.9 Mon 12:15 H16

Investigation of excitonic resonances in monolayer MoSe2 for strong coupling experiments at room temperature — •Nils Lundt[1], Aleksander Maryński[2], Grzegorz Sek[2], Oliver Iff[1], Sefaattin Tongay[3], Sven Höfling[1,4], and Christian Schneider[1] — [1]Chair for Apllied Physics, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Physics, Wrocław University of Technology, Wybrzeze Wyspiańskiego 27, 50-370 Wrocław, Poland — [3]School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, Arizona 85287, United States — [4]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY 16 9SS, United Kingdom

We studied the temperature evolvement of the reflectivity of a MoSe2 monolayer. From this investigation we deduced the dependence of linewidth and oscillator strength on temperature. The results were used for transfer matrix simulations of strong coupling reflectivity spectra, expected if the MoSe2 monolayer is integrated into a micro-cavity. These calculations should evaluate, if strong coupling can be observed in MoSe2 monolayers at room temperature. Calculations were conducted for different cavity designs such as an open cavity approach, a monolithic cavity and for the coupling to a Tamm Plasmon. Moreover, we present results of excitation power dependent photoluminescence studies on MoSe2 monolayers.

O 10.10 Mon 12:30 H16

Localized states from WSe_2 as promising candidates for new single-photon sources — •Sven Borghardt[1], Jhih-Sian Tu[1], Florian Winkler[2], Detlev Grützmacher[1], and Beata Kardynal[1] — [1]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [2]ER-C, Forschungszentrum Jülich, Jülich, Germany

An emission of single photons from WSe_2 monolayers (ML) has been recently demonstrated but the origin of the emission is still not clear. The aim of our research is to understand its origin and then control the localized emission in this material to harvest the unique properties of the material for new applications in quantum photonics.

Samples prepared by exfoliation from synthetic crystals and also grown with CVD are measured using polarization resolved μ-photoluminescence (PL) as well as time-resolved PL.

Our results show linearly polarized emission doublet lines with an energy splitting of up to a few meV. The samples show a high density of such lines close to the sample edges. We attribute the linear polarization of the localized states to a mixing of K- and K'-states. There is an evidence of an alignment of the polarization of emission with the crystal lattice. PL from the localized states decays faster with the temperature than the one from the free exciton states. Chemical modification of the samples is further used in an attempt to manipulate the emission from the localized states.

O 10.11 Mon 12:45 H16

Theoretical studies of transition metal dichalcogenides for the use in electron holography — •Sven Borghardt[1], Zeila Zanolli[4], Matthieu Verstraete[3], Florian Winkler[2], Juri Barthel[2], Rafal Dunin-Borkowski[2], and Beata Kardynal[1] — [1]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [2]ER-C, Forschungszentrum Jülich, Jülich, Germany — [3]PCPM, Université Catholique de Louvain, Louvain-la-Neuve, Belgium — [4]PGI-2 and IAS, Forschungszentrum Jülich, Jülich, Germany

Few-layer transition metal dichalcogenides (TMDs) represent a new family of materials with promising properties for new optoelectronic nano-devices. Their well-known and tailorable thickness render them an ideal system for quantitative electron holography.

Here, we present the simulation of the effect of charge reorganisation due to bonding on the phase acquired by electrons passing through few layer TMD structures in electron holography experiments. This is done by simulating the phases for potentials from density functional theory calculations in comparison with ones obtained from the independent-atom approximation. The results show in an impressive way that neglecting the atomic bonding and the associated small change in the overall charge distribution leads to an overestimation of the average electron phase by approximately 5% for the analyzed materials. Comparison with experimental data confirms this conclusion.

Building on the results for pristine materials, we present calculations for single defects and heterostructures composed of different materials from the transtition-metal dichalcogenide family.