DS 20: 2D materials: Chalcogenides I (joint session HL/DS)

Time: Wednesday 9:30–13:15 Location: A 151

DS 20.1 Wed 9:30 A 151

Theory of Strain-Induced Confinement in Transition Metal Dichalcogenide Monolayers — •Matthew Brooks and Guido Burkard — Universität Konstanz, Konstanz

Recent experimental studies of out-of-plane straining geometries of transition metal dichalchogenide (TMD) monolayers have demonstrated sufficient band gap renormalisation for device application such as single photon emitters. Here, a simple continuum-mechanical plate-theory approach is used to estimate the topography of TMD monolayers layered atop nanopillar arrays. From such geometries, the induced conduction band potential and band gap renormalisation is given, demonstrating a potential shape that is independent of the height of deforming nanopillar. Additional, with a semi-classical WKB approximation, the expected leakage of the strain potential may be estimated as a function of the height of the deforming nanopillar. This straight forward approach is in accordance with experiment, supporting recent findings suggesting that nanopillar height improves linewidth of the single photon emitters observed at the tip of the pillar, yet has no discernible influence over the wavelengths of the emitted photons.

DS 20.2 Wed 9:45 A 151

the role of dark exciton states in magneto-exciton valley depolarisation mechanisms In monolayer transition metal dichcalcogenides — •Alexander Pearce and Guido Burkard — Universität Konstanz, Konstanz, Germany

We present a theoretical study of the valley magneto-exciton relaxation dynamics in monolayer transition metal dichcalcogenides (TMDs) using a kinetic equation approach. The TMDs are direct band gap semiconductors with strong light-matter coupling which produce optical responses dominated by tightly bound excitons. The combination of the lattice symmetry and strong spin-orbit interaction gives rise to a rich selection rules allowing for optical control of the excitons valley polarisation. Experiments have shown that due to spin-orbit interactions there are spin forbidden transitions which lead to dark exciton states, and these states are found to possess long lifetimes due to their non-radiative decay and play a role in the depolarisation dynamics of the TMDs. Using a kinetic equation approach we investigate the interplay of the exchange interaction, a perpendicular magnetic field and the dark state scattering the time evolution of the exciton valley polarisation. We find that the influence of the dark states leads to longer valley relaxation times. We also explore the effect of an in-plane magnetic, which acts to "brighten" the dark states, which leads to an even greater increase in the valley relaxation time.

DS 20.3 Wed 10:00 A 151

Strain on molybdenum disulfide sheets with defects from first principles — •Mohammad Bahmani[1], Mahdi Faghihnasiri[2], and Thomas Frauenheim[1] — [1]BCCMS, Physics Department, Bremen University, Bremen, Germany — [2]Physics Department, Shahrood University of Technology, Shahrood, Iran

Single layer of transition metal dichalcogenides(TMDCs) are under intense investigations since the discovery of unique characteristics of 2D and Vann der Waals layered materials. They are predicted to be the most promising structure for various future nanoscale devices. They have also novel applications in spintronic and optoelectronic.

As a result of thermal equilibrium and the kinetics of processing, all real materials contain structural defects which show significant effects on their electrical, optical, vibrational, magnetic, and chemical properties. Besides, mechanical strain has very much influence on the electronic properties of 2D materials, particularly TMDCs. For example, 0.5% biaxial strain force direct band gap in molybdenum disulfide(MoS2) to become indirect since it breaks the crystalline symmetry.

Therefore, I study different types of point defects such as single and double sulfur(S), single molybdenum(Mo) vacancies, and removing a Mo with its three upper S neighbors. I also substitute a Mo vacancy with one and two S atoms. Furthermore, as the second aim of this study, I showed the modification of defect states under uniaxial and biaxial compression and tensile strain. For the case of one S vacancy, this moves shallow states into the valance band and importantly breaks the degeneracy of degenerate states.

DS 20.4 Wed 10:15 A 151

Optical absorption of a mechanically strained WSe_2 monolayer — •Iris Niehues[1], Robert Schmidt[1], Robert Schneider[1], Matthias Drüppel[2], Torsten Deilmann[2], Michael Rohlfing[2], Steffen Michaelis de Vasconcellos[1], Andres Castellanos-Gomez[3], and Rudolf Bratschitsch[1] — [1]Physikalisches Insitut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [3]Materials Science Factory, Instituto de Ciencia de los Materials de Madrid (ICMM-CSIC), E- 28049 Madrid

Atomically thin layers of transition metal dichalcogenides represent a new class of materials. Strain engineering allows to tune their fundamental optical transitions. We apply reversible uniaxial tensile strain of up to 1.4% to a WSe_2 monolayer. At increasing and decreasing tensile strain levels absorption spectra are recorded, and the strain-dependent energy shifts of the exciton resonances are measured[1]. Gauge factors of $-54\,\mathrm{meV/\%}$, $-50\,\mathrm{meV/\%}$, $+1\ \mathrm{meV/\%}$, and $-22\,\mathrm{meV/\%}$ are derived for the A, B, C, and D exciton, respectively. A comparison with ab initio *GW*-BSE calculations shows an excellent agreement with the measured data.

[1] R. Schmidt, I. Niehues, R. Schneider, M. Drüppel, T. Deilmann, M. Rohlfing, S. Michaelis de Vasconcellos, A. Castellanos-Gomez, and R. Bratschitsch, Reversible uniaxial strain tuning in atomically thin WSe_2 in: 2D Materials 3, 021011 (2016)

DS 20.5 Wed 10:30 A 151

Tunable electron-phonon interaction in MoS2 — •Max Bommert[1], Bastian Miller[1,2], Alexander Holleitner[1,2], and Ursula Wurstbauer[1,2] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 Munich, Germany

Transition metal dichalcogenides such as MoS2 are of current interest for optoelectronic application, as well as for studying fundamental aspects of light-matter interaction and excitonic properties in strictly two-dimensional semiconductors. We explore the impact of the charge carrier density on the electron phonon interaction by non-resonant and resonant Raman spectroscopy. We utilize MoS2 field effect structures with solid electrolyte and liquid ion gates, enabling a change of the 2D electron density by more than two orders of magnitude [1]. We report unusual polarization and charge carrier dependent behavior in resonant Raman spectra that points towards strong electron-phonon coupling in MoS2 and the importance of excitonic phenomena [2]. Alongside we investigate temperature dependent phase transitions through changes in transport and optical properties.

[1] Miller et al., APL 106, 122103 (2015)
[2] Miller, Bommert et al. (2018)

DS 20.6 Wed 10:45 A 151

Theory of Exciton-Exciton Interactions in Monolayer Transition Metal Dichalcogenides — •Florian Katsch, Malte Selig, Alexander Carmele, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik von Halbleitern, Technische Universität Berlin, 10623 Berlin, Germany

Due to the strong Coulomb interaction in monolayers of transition metal dichalcogenides (TMDs), the optical properties are governed by tightly bound electron-hole pairs in the vicinity of the band edge. In order to allow for efficient modeling, a theoretical description in a two particle exciton basis based on the unit-operator method [1] is introduced. The formalism incorporates TMD-typical Coulomb inter- and intravalley interactions up to three correlated excitons. The developed theory is applied to access the exciton dynamics [2,3] in the so-called coherent limit as well as exciton-phonon interactions [4]. The derived TMD Bloch equations contribute to the understanding of recent pump-probe experiments observing an immediate signal in the unpumped valley [5,6].

[1] A. L. Ivanov and H. Haug, *Physical Review B* **48**, 1490 (1993).
[2] V. M. Axt and A. Stahl, *Zeitschrift für Physik B Condensed Matter* **93**, 2 (1994).
[3] M. Lindberg et. al., *Physical Review B* **50**, 18060 (1994).
[4] M. Selig et. al., *Nature communications* **7**, 13279 (2016).

[5] C. Mai et. al., *Nano letters* **14**, 202 (2013).
[6] R. Schmidt et. at., *Nano letters* **16**, 2945 (2016).

DS 20.7 Wed 11:00 A 151

Optical spectra and bound excitons in MoTe2 from monolayer to bulk by many-body perturbation theory — •Saeideh Edalati-Boostan, Caterina Cocchi, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Among the transition-metal dichalcogenides, MoTe2 plays a relevant role as a good candidate for light-emitting devices. In the framework of GW and the Bethe-Salpeter equation as implemented in the exciting code [1], we study optical excitations in this material as a function of dimensionality, going from mono- and bilayers to the bulk. The role of spin-orbit coupling is assessed in band structures and optical spectra with respect to the number of layers. The calculated absorption spectra are characterized by a few bound excitons in the visible region with binding energies of the order of a hundred meV [2]. Bound electron-hole pairs, which are known to be both inter- and intra-layer in bulk MoTe2 [2], are analyzed in view of quantum confinement effects. This understanding is essential to eventually use this material in van der Waals heterostructures.

[1] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, and C. Draxl, JPCM 26, 36 (2014); D. Nabok, A. Gulans, and C. Draxl, PRB 94, 035118 (2016); S. Sagmeister, and C. Draxl, PCCP 11, 4451 (2009)

[2] A. Arora, M. Drüppel, R. Schmidt, T. Deilmann, R. Schneider, M. R. Molas, Ph. Marauhn, S. M. de Vasconcellos, M. Potemski, M. Rohlfing, and R. Bratschitsch, Nat Commun. 8, 639 (2017)

15 min. break.

DS 20.8 Wed 11:30 A 151

Thermal annealing effects on optical properties of 2D MoS_2 — •Oleg Gridenco, Kathrin Sebald, Christian Tessarek, Martin Eickhoff, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, Germany

Mechanically exfoliated monolayers obtained by using natural crystals and deposited by a polymer transfer process on substrates suffer from residues on the surface which are hard to be removed. The residues as well as absorbed O_2 and H_2O at the surface of a monolayer are known to modify the optical and electrical properties resulting in a quenching of the photoluminescence (PL) and a reduction of the carrier mobility. We present a systematic thermal annealing study conducted by heating and laser annealing in order to remove such residues. The results show that the PL energy is blue-shifted and the PL intensity is enhanced by a factor of 1.8 after a thermal annealing cycle. The blue-shift points to a reduction of the trion contribution and a relative increase of free-exciton recombination. In addition, the overall PL enhancement can be related to a decrease of non-radiative recombination processes. A similar behaviour of the PL is observed after MoS_2 monolayers were exposed to UV laser irradiation for several seconds. The study provides a low-cost, large scale and effective route to enhance the PL efficiency which is important for the device performance.

DS 20.9 Wed 11:45 A 151

Spatiotemporal dynamics of the carrier capture into localized states in a TMDC monolayer — •Roberto Rosati, Frank Lengers, Doris E. Reiter, and Tilmann Kuhn — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Monolayers of transition metal dichalcogenides (TMDC) have attracted wide attention due to their interesting optical and electronic properties. Local strain distributions lead to the formation of embedded 0D confinement potentials which can be exploited, e.g., as single photon sources [1]. In such hybrid 2D-0D systems, the bound states of the 0D potential may be populated through carrier capture by emission of optical phonons. Such capture processes are known to generate non-trivial spatiotemporal dynamics in hybrid 1D-0D systems [2]. In this work we study the capture of a wave packet in a MoSe2 monolayer into localized states. We find interesting spatio-temporal dynamics of the trapped charge distribution associated with the capture into specific superposition states, which can be controlled by the propagation direction of the wave packet. To calculate the dynamics we use a recently introduced Lindblad single-particle approach, which allows us to deal with the dimensionality-related computational demands and, at the same time, catches the most relevant features of the carrier capture, in particular its locality [3].

[1] Kern et al., Adv. Mater., **28**, 7101-7105 (2016)
[2] Glanemann et al., Phys. Rev. B **72**, 045354 (2005)
[3] Rosati et al., Phys. Rev. B **95**, 165302 (2017)

DS 20.10 Wed 12:00 A 151

Strong Anisotropic Spin-Orbit Interaction Induced in Graphene by Monolayer WS_2 — •Taro Wakamura[1], Francesco Reale[2], Pawel Palczynski[2], Cecilia Mattevi[2], Sophie Guéron[1], and Hélène Bouchiat[1] — [1]Laboratoire de Physique des Solides, Université Paris-Sud, Orsay, France — [2]Department of Materials, Imperial College London, London, United Kingdom

We demonstrate strong anisotropic spin-orbit interaction in graphene induced by monolayer WS2. Direct comparison between graphene/monolayer WS2 and graphene/bulk WS2 system in magnetotransport measurements reveals that monolayer transition metal dichalcogenide can induce much stronger SOI than bulk. Detailed theoretical analysis of the weak-antilocalization curves gives an estimated spin-orbit energy (Eso) more than 10 meV. The dominant z to -z symmetric spin-orbit interaction demonstrates strong valley-Zeeman spin-orbit interaction induced in graphene, consistent with the recent theoretical study. Dramatic increase of resistance around the Dirac point with decreasing temperature suggests the existence of the spin-orbit gap at the Dirac point.

DS 20.11 Wed 12:15 A 151

Electronic and optical properties of group-IV transition metal dichalcogenides monolayers and their heterostructures — •Ka Wai Lau, Caterina Cocchi, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

The interest in transition-metal dichalcogenides (TMDs) monolayers as promising materials for opto-electronics has rapidly increased in the last few years [1]. The majority of studies has been devoted so far to group-VI TMDs, with MoS2 and WS2 as the most relevant examples of this material class [1]. Here, we study monolayers of group-IV TMDs focusing on ZrS2 and HfS2. We investigate their electronic and optical properties in the framework of many-body perturbation theory (GW and the Bethe-Salpeter equation) as implemented in the all-electron full-potential code exciting [2]. The optical response of these systems is characterized by intense peaks in the visible region due to tightly-bound excitons with binding energies of the order of hundreds of meV. The degeneracy of the hole state at the Γ point with different dispersion along the M-Γ-K direction and the strong spin-orbit coupling in the valence band leads to several distinct excitonic states around Γ. Finally we study van-der-Waals heterostructures obtained by combining ZrS2 and HfS2 monolayers in view of understanding how different stacking patterns influence band alignment and optical excitations.

[1] K. F. Mak and J. Shan, Nat. Photon. 10, 216 (2016)
[2] A. Gulans et al., J. Phys.: Condens. Matter 26, 363202 (2014)

DS 20.12 Wed 12:30 A 151

Persistent photoconductivity in monolayer MoS_2 field effect transistors after UV irradiation — •Antony George[1], Mikhail Fistul[2,3], Uwe Hübner[4], Nirul Masurkar[5], David Kaiser[1], Christof Neumann[1], Andreas Winter[1], Arava Leela Mohana Reddy[5], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, 07743 Jena, Germany — [2]Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon 34051, Republic of Korea — [3]Russian Quantum Center, National University of Science and Technology "MISIS", 119049 Moscow, Russia — [4]Leibniz Institute of Photonic Technology, 07745 Jena, Germany — [5]Department of Mechanical Engineering, Wayne State University, 48202 Detroit, USA

We demonstrate long living photo-excited charge carriers in monolayer MoS_2 field effect transistors (FET) after UV irradiation. After irradiation, the FETs were found to be remaining in a high conductivity state at room temperature (RT) for a long time (ca. 30 days). We investigated the origin of the persistent photoconductivity (PPC) combining RT and low-temperature transport measurements with theoretical modeling. At low temperatures, a great enhancement of photo-induced conductivity with applied gate voltage was observed. We ascribe this to the UV irradiation of MoS_2, which results in inter-band transitions and the creation of a large number of electron-hole pairs, which are quickly spatially separated due to local variations of the band structure. Under such conditions, the recombination time drastically increases and

induces the PPC effect.

DS 20.13 Wed 12:45 A 151

Highly polarized excitons in atomically thin and bulk-like 1T'-ReSe$_2$ — •A. Arora[1], J. Noky[2], M. Drüppel[2], B. Jariwala[3], T. Deilmann[4], R. Schneider[1], R. Schmidt[1], O. Del Pozo-Zamudio[1], T. Stiehm[1], A. Bhattacharya[3], P. Krüger[2], S. Michaelis de Vasconcellos[1], M. Rohlfing[2], and R. Bratschitsch[1] — [1]Institute of Physics, University of Münster, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany — [2]Institute of Solid State Theory, University of Münster, D-48149 Münster, Germany — [3]Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400005, India — [4]Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Using low-temperature polarized optical absorption and photoluminescence spectroscopy, supported by GW-BSE ab initio calculations, we investigate excitons in the van der Waals semiconductor 1T'-ReSe$_2$ [1]. A red shift of the excitonic transition energy is observed when the crystal thickness is reduced from bulk towards a monolayer. The excitons exhibit a strong polarization anisotropy within the plane of the crystal, with dipole vectors pointing towards different crystal directions. This polarization behavior persists from bulk to monolayer thickness. We find that the excitons are strongly confined within the individual crystal layers, even for the bulklike case. We find a direct band gap in 1T'-ReSe$_2$ in our calculations, regardless of the crystal thickness. Our results pave the way for polarization-sensitive applications using two-dimensional semiconductors. [1] A. Arora et al., Nano Lett. 17, 3202-3207 (2017).

DS 20.14 Wed 13:00 A 151

The Influence of the environment on monolayer tungsten diselenide photoluminescence — •Lorenz Maximilian Schneider[1], Sina Lippert[1], Jan Kuhnert[1], Obafunso Ajayi[2], Dylan Renaud[1], Young Duck Kim[2,3], Wolfram Heimbrodt[1], James C. Hone[2], and Arash Rahimi-Iman[1] — [1]Department of Physics and Material Sciences Center, Philipps-Universität Marburg, 35032 Marburg , Germany — [2]Department of Mechanical Engineering, Columbia University, 10027 New York, USA — [3]Department of Physics and Center for Humanities and Sciences, Kyung Hee University, 02447 Seoul, Republic of Korea

In recent years, two-dimensional (2D) semiconductors have drawn a lot of attention due to their special properties. Since transition metal dichalgogenides (TMDs) are a potential candidate for opto-electronic applications in the visible range, they are of major interest and subject of many studies. Recent investigations have shown that encapsulating monolayers with hBN can improve signal quality greatly compared to flakes grown or exfoliated on common substrates. Here, we present a systematic study of the effects, that such encapsulation of monolayers with mainly hBN can have on the 2D material's optical properties using WSe_2. Besides the already known narrowing of the PL-linewidth, remarkable differences are found in the time evolution. hBN supported and encapsulated samples show a significantly stronger exciton-exciton annihilation as the reference samples on bare substrate. Furthermore, we show that this effect is also obtained if the heterostructure consists of two TMDs.