DS 28: 2D materials: Chalcogenides II (joint session HL/DS)

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

DS 28.1 Thu 9:30 A 151

Excitation-induced transition from direct to indirect band gaps in monolayer TMDCs — •Daniel Erben[1], Alexander Steinhoff[1], Tim Wehling[1,2], Christopher Gies[1], and Frank Jahnke[1] — [1]Insitute for Theoretical Physics, University of Bremen, Germany — [2]Bremen Center for Computational Materials Science, University of Bremen, Germany

Monolayer transition metal dichalcogenides (TMDCs) are atomically thin semiconductors with a direct band gap, which allows their use as active material in optoelectronic devices. Often photoluminescence or photoemission spectroscopy experiments are employed for the characterization of TMDCs. Via laser pulse excitation these methods provide excited charge carriers that populate the valleys of the band structure. The Coulomb interaction of these excited carriers causes strong many-body renormalizations in the band structure, which consequently shift the valleys and the excitonic resonances by several hundred meV.
In this talk we give detailed insight into the many-body effects in monolayer MoS_2, $MoSe_2$, WS_2 and WSe_2 by evaluating the semiconductor Bloch equations including DFT-band structures and interaction-matrix elements. This provides a precise description for the interplay of the Coulomb interaction with the electron and hole populations. We describe the impact of these effects on the K- and Σ-valley in the band structure. Our calculations show a clear tendency to a direct-to-indirect band gap transition due to the renormalizations. Being reminiscent of the effect of strain on monolayers, this transition should also lead to a quenching of the photoluminescence.

DS 28.2 Thu 9:45 A 151

Microscopic description of localized quantum-dot-like states in MoS2 nanobubbles — •Christian Carmesin, Matthias Florian, Michael Lorke, Daniel Erben, and Frank Jahnke — Institute for Theoretical Physics, University of Bremen, Germany

Atomically thin layers of transition metal dichalcogenides (TMDCs) have emerged as a new class of optically active materials with recent applications reaching into the quantum-information technologies. The systematic engineering of local confinement potentials opens the possibility of the deterministic generation of single-photons. A possible platform are TMDC nanobubbles that develop if air is enclosed during the stacking of layers. We report on results of atomistic tight-binding calculations of different sizes and height-to-diamter ratios of these nanostructures and show that the formation of confined quantum-dot-like single-particle states is caused by an interplay of strain and dielectric screening.

DS 28.3 Thu 10:00 A 151

Optical properties of TMDC semiconductors in the 1,55μm telecom wavelength range — •Michael Lorke and Frank Jahnke — Institute für theoretische Physik, Universität Bremen

In the context of the current interest in atomically thin semiconductors, we study optical properties of highly excited and/or highly doped transition-metal dichalcogenides (TMDCs). We show that under such excitation conditions, transitions between the first and higher conduction bands are possible. These transitions are analogous to intersubband transitions in conventional quantum well devices. In this work we discuss the carrier density and temperature dependence of such transitions and show that they can be tuned into the technologically relevant 1,55μm telecom wavelength range. This opens the possibility to utilize TMDCs in novel devices ranging from quantum cascade lasers to novel infra-red photodetectors.

DS 28.4 Thu 10:15 A 151

Coupling of a monolayer of WSe2 to an InGaP bullseye cavity — •Oliver Iff[1], Vasilij Baumann[1], Monika Emmerling[1], Marcelo Davanco[2], Kartik Srinivasan[2], Sven Hoefling[1,3], and Christian Schneider[1] — [1]Technische Physik, Universitaet Wuerzburg, Am Hubland, Wuerzburg, Germany — [2]Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, Maryland, U.S.A. — [3]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, UK

Photonic cavities based on circular gratings can be used to enhance the emission of optically active materials. Here, we investigate the optical properties of such a cavity consisting of centric rings of InGaP which are completely surrounded by air, forming a floating membrane. The characterization was done via photoluminescence measurements using embedded quantum dots as light source and spatially mapping out the near field emission. Strikingly, the grating membrane can also be transferred via the dry-stamp method onto a given substrate without disturbing its optical modes and therefore opening up new ways of building coupled systems. Furthermore, the structures are optimized for wavelengths near 750nm, making it suitable for coupling to different kinds of 2D materials like WSe2 or MoSe2. A monolayer of WSe2 has been transferred onto the cavity showing improved photoluminescence of the charged exciton right at the centre position. This enables a new path to couple monolayer of 2D materials to photons in order to gain access to quantum electrodynamic effects including strong light-matter coupling.

DS 28.5 Thu 10:30 A 151

Exciton-phonon coupling in mono- and bilayer $MoTe_2$ — •Sophia Helmrich[1], Robert Schneider[2], Alexander W. Achtstein[1], Ashish Arora[2], Bastian Herzog[1], Steffen Michaelis de Vasconcellos[2], Mirco Kolarczik[1], Oliver Schöps[1], Rudolf Bratschitsch[2], Ulrike Woggon[1], and Nina Owschimikow[1] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany — [2]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany

We investigate excitonic transitions of mechanically exfoliated monolayer and bilayer molybdenum ditelluride ($MoTe_2$) by temperature-dependent photoluminescence spectroscopy. Based on identical scaling of the excitonic optical bandgap and the integrated area of the emission with temperature we conclude that ML and BL $MoTe_2$ have similar band alignment and excitonic behavior. Our experiments show that for identical excitation laser power the bilayer yields twice the intensity as the monolayer unlike for other transition metal dichalcogenides. From the emission lines we extract key parameters for exciton-phonon coupling processes demonstrating an unusually small coupling with acoustical phonons of $\gamma_{\mathrm{LA}} = (28 \pm 4)\,\mu\mathrm{eV\,K^{-1}}$ and $(14 \pm 4)\,\mu\mathrm{eV\,K^{-1}}$ for ML and BL $MoTe_2$, respectively, where the interactions with longitudinal optical phonons of $\Gamma_{LO} = (40.1 \pm 5.6)$ meV ((86.4 ± 12.6) meV) for ML (BL) $MoTe_2$ are comparable to values of other TMDs. These observations make $MoTe_2$ an attractive and robust material with a large luminescence yield for applications in the technically relevant near-infrared region.

DS 28.6 Thu 10:45 A 151

Giant Gap-Plasmon Tip-Enhanced Raman Scattering of MoS2 Monolayers on Au Nanocluster Arrays — •Mahfujur Rahaman[1], Alexander G. Milekhin[2,3], E. E. Rodyakina[2,3], A. V. Latyshev[2,3], Volodymyr M. Dzhagan[1,4], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107, Chemnitz, Germany — [2]Novosibirsk State University, Pirogov 2, 630090, Novosibirsk, Russia — [3]Rzhanov Institute of Semiconductor Physics RAS, Lavrentiev Ave. 13, 630090, Novosibirsk, Russia — [4]V. Lashkaryov Institute of Semiconductors Physics, Nat. Acad. of Sci. of Ukraine, 03028, Kyiv, Ukraine

We present the results on a gap-plasmon tip-enhanced Raman scattering study of MoS2 monolayers deposited on a periodic array of Au nanostructures on a silicon substrate forming a two dimensional (2D) crystal / plasmonic heterostructure. We observe a giant Raman enhancement of the phonon modes of the MoS2 monolayer located in a plasmonic gap between Au tip apex and Au nanoclusters. Tip-enhanced Raman (TER) mapping allowed us to determine the gap-plasmon field distribution responsible for the formation of hot spots. These hot spots provided an unprecedented giant Raman enhancement of 5.6 * 108 and a spatial resolution as small as 2.3 nm at ambient conditions. Moreover, due to strong hot electron doping in the order of 1.8 * 1013 cm-2, we observed a structural change of MoS2 from 2H to 1T phase. Thanks to the very good spatial resolution, we were able to spatially resolve those doping sites. Our results open the perspectives of optical diagnostics in nanoscale for many other 2D materials.

DS 28.7 Thu 11:00 A 151

Doping dependent photoluminescence of ML WSe2 — Jhih-Sian Tu, •Sven Borghardt, Detlev Grützmacher, and Beata Kardynał — Peter Grünberg Institute 9 (PGI-9), Forschungszentrum

Jülich, Germany

While free exciton states of monolayer transistion meatal dichalcogenides are well understood, photoluminescence spectra of WSe_2 contain number of low energy features that are not understood and collectively referred to as localized states. Such signal is not observed in spectra of materials with the lowest energy state being bright for example in the spectra of monolayer MoSe_2. In order to shed light on the origin of the sub-bandgap emission from WSe_2, we measured low temperature photoluminescence at a very wide range of both electron and hole doping levels. The spectra appear rich in structure which is very strongly doping dependent. The spectral, polarization and spatial correlations between the long wavelength emission features with the signal from the recombination of the bright exciton and trion states are consistent with the brightening of momentum-dark states either by phonon-mediated processes or by interactions of excitons with electrons or plasmons. Unexpectedly, while majority of the spectral features share polarization properties of excitons and trions, some show cross-polarization with the excitation laser.

15 min. break.

DS 28.8 Thu 11:30 A 151

Effective theory of monolayer TMDC double quantum dots — •Alessandro David, Andor Kormányos, and Guido Burkard — Department of Physics, University of Konstanz, D-78464, Germany

Monolayer Transition Metal Dichalcogenides (TMDCs) are promising candidates for the creation of quantum dots, because they are truly two-dimensional semiconductors with a direct band gap. One of their features is an intrinsic spin-orbit interaction that splits the spins in the conduction and valence band. In this work, we analyse theoretically the behaviour of a double quantum dot (DQD) system created in the conduction band of these materials, with two electrons in the regime of the (1,1) charge configuration. Motivated by recent experimental progress, we consider several scenarios, such as when the spin splitting is different in the two dots or when the the valley degeneracy in the TMDC is removed due to a ferromagnetic insulator substrate. Finally, we discuss in which cases it is possible to reduce the low energy subspace to the lowest Kramer's pairs, where novel interactions appear.

DS 28.9 Thu 11:45 A 151

transport properties of high-quality ultrathin two-dimensional superconducting Mo2C crystals and Heterostructures — •n. kang[1], l.b wang[1], c. xu[2], s. song[1], and w.c. ren[2] — [1]Peking University, Beijing, P. R. China. — [2]Institute of Metal Research, Shenyang, P. R. China.

There is particularly interesting in the studies on highly crystalline 2D superconductors. Recently, we have obtained high-quality ultrathin Mo2C crystals and graphene/Mo2C heterostructures by means of chemical vapor deposition method [1-3]. Here, we report on transport measurements on superconducting Mo2C crystals and heterostructures in the 2D limit. We observe magnetoresistance (MR) oscillations and negative MR at low magnetic fields for temperature far below superconducting transition temperature[2,3]. We discuss that these anomalous behaviors can be understood quantitatively by including the effects of inhomogeneous superconducting phase and quantum fluctuations. For graphene/ Mo2C heterostructures, we demonstrate the realization of highly transparent Josephson junction devices based on these strongly coupled heterostructures[3].

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[2] L. B. Wang, C. Xu, Z. B. Liu, L. Chen, X, L. Ma, H. M. Cheng, W. C. Ren*, and N. Kang*, ACS NANO, 10, 4504(2016).

[3] C. Xu, S. Song, Z. B. Liu, L. Chen, L. B. Wang, D. X. Fan, N. Kang*, X, L. Ma, H. M. Cheng, and W. C. Ren*, ACS NANO, 11, 5906 (2017).

DS 28.10 Thu 12:00 A 151

Nanoplatelets - a material system between strong confinement and weak confinement — •Marten Richter — Institut für Theoretische Physik, Technische Universität Berlin, Germany

Recently grown CdSe Nanoplatlets are often described to have a similar electronic structure as two-dimensional quantum wells and are promoted as colloidal quantum wells with monolayer precision width. Here we show, that nanoplatelets are not ideal quantum wells, but cover (depending on their size a strong confinement) an intermediate and a Coulomb interaction dominated regime [1]. For the analysis we show results from a solution of the full four dimensional exciton wave function and analyze different confinement regimes.

[1] Phys. Rev. Materials 1, 016001 (2016)

DS 28.11 Thu 12:15 A 151

Giant magnetic splitting inducing near-unity valley polarization in van der Waals heterostructures — •Philipp Nagler[1], Mariana V. Ballottin[2], Anatolie A. Mitioglu[2], Fabian Mooshammer[1], Johannes Holler[1], Jonas Zipfel[1], Michael Kempf[1], Nicola Paradiso[1], Christoph Strunk[1], Rupert Huber[1], Alexey Chernikov[1], Peter C. M. Christianen[2], Christian Schüller[1], and Tobias Korn[1] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]High Field Magnet Laboratory (HFML), Radboud University, The Netherlands

Atomically thin van der Waals heterostructures enable solid-state systems in the ultimate thickness limit. Type II band alignment of transition metal dichalcogenides (TMDCs) leads to the formation of interlayer excitons, which stem from spatially separated electron-hole pairs. These species are highly promising for future valleytronic devices since they combine ultra-long lifetimes with the peculiar spin-valley physics of the constitutent monolayers. Here, we demonstrate strong magnetic coupling of interlayer excitons in a $WSe_2/MoSe_2$ heterostructure to an external magnetic field up to 30 T. The observed g factor of -15 by far exceeds typical values of the g factor in TMDC monolayers and enables near-unity valley polarization of long-lived interlayer excitons at high fields. Our findings can be made plausible by taking into account the AB-stacking configuration of the heterostructure where K+ and K− valleys align in momentum space, leading to spin-allowed inter-valley optical transitions.

DS 28.12 Thu 12:30 A 151

Effective passivation of ultra-thin layers of InSe to enhance electrical properties — •Himani Arora[1,2], Younghun Jung[3], Sanghoon Chae[3], Daniel Rhodes[3], Ghidewon Arefe[3], Takashi Taniguchi[4], James Hone[3], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Department of Mechanical Engineering, Columbia University, New York, NY, 10027, USA — [4]Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

We report electrical properties of ultrathin layers of Indium Selenide (InSe), a member of the III-VI chalcogenides family, which has shown a mobility two orders of magnitude higher than MoS2, alongside better stability than black phosphorus.

InSe has light electron effective mass and high mobility enabling its usage for fast, high performance electronics. State-of-the-art InSe transistors reported so far, consist of 6 nm thick InSe flake contacted using graphene edge contacts and reaching a mobility of 1500 cm2V-1s-1 at RT in top-gate configuration. However, InSe being an air-sensitive material loses its conductance over time, resulting the transistor to become unfunctional.

In this study, we report an InSe-based transistor fully encapsulated in h-BN layers which enhanced its electrical properties compared to an un-encapsulated device. The transistor reached a high Hall mobility at RT, while retaining its performance for a long period of time.

DS 28.13 Thu 12:45 A 151

Impact of layer separation on the optoelectronic properties of van der Waals heterostructures — •Malte Hartmann[1], Matthias Florian[1], Alexander Steinhoff[1], Frank Jahnke[1], Julian Klein[2], Alexander Holleitner[2], Jonathan Finley[2], Tim Wehling[1], Michael Kaniber[2], and Christopher Gies[1] — [1]Institut für theoretische Physik, Bremen, Deutschland — [2]Walter Schottky Institut, München, Deutschland

Dielectric screening plays an important role in the field of atomically thin transition-metal dichalcogenides (TMDs) and van der Waals heterostructures consisting of stacked 2D-materials. In each layer the field lines of the Coulomb interaction are screened by the adjacent material, which reduces the single-particle band gap as well as binding energies of exciton complexes and can be used to tailor the optoelectronic properties. By combining an electrostatic model for a dielectric hetero-multi-layered environment with semiconductor many-particle methods, we demonstrate that the electronic and optical properties are sensitive to the interlayer distances on the atomic scale. Spec-

troscopical measurements in combination with a direct solution of a three-particle Schrödinger equation reveal trion binding energies that correctly predict recently measured interlayer distances.

DS 28.14 Thu 13:00 A 151

Band Gaps and Carrier Relaxation in Thin Films of ZrS_3 — •Christopher Belke[1], Sonja Locmelis[2], Johannes C. Rode[1], Hennrik Schmidt[1], Bastian Hoppe[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

New varieties of two-dimensional crystals [1] are currently getting into focus of the material sciences. An example for such layered materials are Transition Metal Trichalcogenides. Here we study the compound ZrS_3: bulk crystals were synthesized by chemical gas transport; stoichiometry and structure were verified by powder X-ray diffractometry and energy-dispersive X-ray spectroscopy (EDX), and analyzed by absorption measurements. The latter indicate an indirect bandgap of about 1.8 eV and a direct bandgap of 2.3 eV, which differ slightly from literature values [2, 3]. Thin flakes are exfoliated and contacted. Conductivity measurements are investigated in response to illumination with LEDs of different wavelengths. We observe a pronounced rise in conductivity between 2.1 eV and 2.4 eV which is in good agreement with the direct bandgap found in the absorptions measurements. Measurements of charge carrier relaxation are described by a power-law dependence and reveal unexpectedly long relaxation times.

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[2] M. Abdulsalam, D. Joubert, Eur. Phys. J. B. 88, 177 (2015).
[3] Y. Jin, X. Li, J. Yang, Phys. Chem. Chem. Phys. 17, 18665 (2015).