DS 4: 2D semiconductors and van der Waals heterostructures I (joint session HL/DS/O)

Time: Monday 9:30–13:00 Location: POT 81

DS 4.1 Mon 9:30 POT 81

Demonstration of a broadband Photodetector Based on a Two-Dimensional Metal-Organic Framework — •Himani Arora[1,2], Renhao Dong[3], Tommaso Venanzi[1,2], Jens Zscharschuch[1], Harald Schneider[1], Manfred Helm[1,2], Xinliang Feng[3], Enrique Cánovas[4], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Faculty of Physics & Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany — [3]Faculty of Chemistry and Food Chemistry & Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany — [4]Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA Nanociencia), 28049 Madrid, Spain

Electrically-conducting metal-organic frameworks (MOFs) have gained considerable attention in last years. In this regard, we report a novel semiconducting Fe3(THT)2(NH4)3 (THT, 2,3,6,7,10,11-triphenylenehexathiol) two-dimensional MOF. The developed MOF films reveal a free-charge band-like transport with a record-high Hall mobility of 230 cm2 V-1 s-1 at room temperature. We further demonstrate a proof-of-concept photodetector based on Fe3(THT)2(NH4)3 MOF films, operative in UV-to-NIR range. Due to IR bandgap of the MOF samples (0.45 eV), the photodetectors are best operated at cryogenic temperatures by suppressing the noise from thermally-activated charge carriers to obtain a clear signal from optically generated carries. Our work reports the first proof-of-concept MOF photodetector, revealing MOFs as promising candidates for optoelectronics.

DS 4.2 Mon 9:45 POT 81

Theory of synchrotron-based spectroscopic techniques on two-dimensional materials — •Dominik Christiansen, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

High energy radiation enables the spectroscopic analysis of core level electronic excitations.

First, we develop a theoretical framework for X-ray absorption spectroscopy (XAS) including electronic and structural information obtained from near-edge XAS and extended XAS [1]. Analysing graphene as exemplary material, we show that the characteristic behaviour of the XAS spectra can be derived from the semi-empirical tight-binding approach by considering the spatially non local light-matter interaction.

Second, we develop a theory of exciton dynamics in time and angle resolved photoemission spectroscopy investigating the exciton formation and thermalization in ultrathin transition-metal dichalcogenides [2,3].

[1] B. Buades *et al.*, Optica **5**, 000502 (2018)
[2] D. Christiansen *et al.*, Phys. Rev. B **100**, 205401 (2019)
[3] M. Selig *et al.*, 2D Mater. **5**, 035017 (2018)

DS 4.3 Mon 10:00 POT 81

The Ultimate Radiative Emission Rate of van der Waals materials — •Mark Kamper Svendsen[1], Yaniv Kurman[2], Ido Kaminer[2], and Kristian Sommer Thygesen[1] — [1]Techincal University of Denmark, Kgs. Lyngby, Denmark — [2]Technion University, Haifa, Israel

We consider the coupling between intersubband transitions in few layer transition metal dichalcogenide(TMD) stacks and graphene plasmons. Specifically, we consider few layer TMD quantum wells[1] of different thicknesses, squeezed in between a metallic substrate and a graphene sheet. Using a new, non-perturbative combined MQE-DFT time domain methodology to calculate the state evolution, we find radiative rates exceeding 1 THz and extreme Purcell factors of more than 1E6. Interestingly, we find that for certain combinations of the TMD stack width and graphene Fermi level, graphene plasmon launching becomes the dominant method of emission. This could potentially point to interesting new possibilities in graphene plasmonics.

[1] Schmidt, P., Vialla, F., Latini, S. et al. Nano-imaging of intersubband transitions in van der Waals quantum wells. Nature Nanotech 13, 1035*1041 (2018) doi:10.1038/s41565-018-0233-9

DS 4.4 Mon 10:15 POT 81

Excitation-induced optical nonlinearities and charge carrier localization in atomically thin TMD semiconductors — •Daniel Erben[1], Alexander Steinhoff[1], Michael Lorke[1,2], Christian Carmesin[1], Matthias Florian[1], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen — [2]BCCMS, University of Bremen

To interpret the nonlinear optical properties of atomically thin transition metal dichalcogenides (TMD), the density of photoexcited carriers is of central importance. However, in experiments the excited carrier density is practically not accessible. For the case of above band-gap optical pumping of TMD monolayers, we utilize the semiconductor Bloch equations to determine the excitation density as function of the optical pump fluence. Our theory includes Pauli-blocking, band-gap renormalization, dephasing and screening of the Coulomb interaction due to excited carriers. The excitation density strongly depends on the wavelength of the exciting laser pulse. For pumping at the band gap, Pauli blocking of available phase space and renormalizations of the single particle energies are the dominant sources of a nonlinear density dependence, even at small pump fluence. In another study, we investigate the charge-carrier confinement in TMD nanobubbles. The latter are formed during stacking processes and exhibit quantum light emission upon optical excitation. We demonstrate that the emission originates from strong carrier localization, which is caused by the interplay of surface wrinkling, strain-induced confinement, and local changes of the dielectric environment. These effects combine to a specific localization signature that is found in recent spatially resolved photoluminescence experiments.

DS 4.5 Mon 10:30 POT 81

Near-field photoluminescence of two-dimensional semiconductors — •Vlastimil Křápek, Petr Dvořák, Martin Konečný, Lukáš Kejík, Michal Horák, and Tomáš Šikola — CEITEC, Brno University of Technology, Purkyňova 123, 61200 Brno, Czech Republic

Layered two-dimensional semiconductors are ideal light sources for on-chip integration. They exhibit strong luminescence even at elevated temperature, are very compact, highly tunable, and capable of single-photon emission. Since the wavelength of the light is considerably larger than the physical dimensions of the emitter, near-field handling of the emission with a deeply subwavelength spatial resolution would be of great importance. Here we present fully near-field photoluminescence experiment of two-dimensional semiconductors, with a surface plasmon interference device (SPID) used for the excitation and scanning near-field optical microscopy (SNOM) for the collection.

A SPID is formed by an opaque gold layer with the thickness of about 200 nm with the subwavelength grooves serving as sources of surface plasmon polaritons (SPP) [1]. We characterize the electric near field of SPP by SNOM, demonstrating the ability of SPP to excite the semiconductor placed on the SPID. We also demonstrate the polarization sensitivity of the experiment [1,2]. Next, we put various layered two-dimensional semiconductors on top of the SPID and characterize their SPP-excited luminescence by SNOM, demonstrating subwavelength spatial resolution.

[1] P. Dvořák et al., Opt. Express **25**, 16560 (2017).
[2] P. Dvořák et al., Nanoscale **10**, 21363 (2018).

DS 4.6 Mon 10:45 POT 81

2D Semiconductors in moving and standing phonon fields — •Tobias M. Petzak, Emeline D. S. Nysten, and Hubert J. Krenner — Lehrstuhl für Experimentalphysik 1, Institut für Physik, Universität Augsburg, Universitätstr. 1, 86159 Augsburg, Germany

In this work, we prepare two-dimensional layers of transition metal dichalcogenides (TMDCs) such as MoS_2, $MoSe_2$, WS_2 or WSe_2 via micromechanical exfoliation and transfer them into the propagation path of a Surface Acoustic Wave (SAW) directly on a $LiNbO_3$ substrate via viscoelastic stamping. The electric field of the SAW couples to the electron system of the monolayer semiconductors and, thus, we gain insight into the dynamics of photogenerated charges in the sample in a non-invasive, completely contact-free, way.

Additionally, we coupled WSe_2 monolayers to the phononic modes of a high quality factor SAW resonator. This resonator-based spectroscopy increases the sensitivity of our technique. In spectrally resolved experiments using the resonator we are able to resolve the ab-

sorption edge of the 2D semiconductor which is in agreement with photoluminescence data. The latter results mark the first major step toward highly sensitive SAW spectroscopy employing SAW resonators.

30 min. break

DS 4.7 Mon 11:30 POT 81

Interlayer excitons in $MoSe_2/WSe_2$ heterobilayers — •Johannes Michl[1], Oliver Iff[1], Maximilian Waldherr[1], Sefaattin Tongay[2], Martin Kamp[1], Sven Höfling[1], and Christian Schneider[1] — [1]Technische Physik, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Arizona State University

Two dimensional materials such as monolayers of transition metal dichalcogenides (TMDs) offer a wide range of possibilities for investigation due to their unique optical properties, resulting from the exotic valley physics and the strong Coulomb interaction. By stacking two different TMDs, a van der Waals heterostructure is formed. This heterobilayer can exhibit a type-II band alignment, enabling formation of interlayer excitons, with the electron and the hole residing in separate layers. As the heterobilayer is formed, spatially periodical moiré potentials occur due to the lattice mismatch and twist of the different monolayer materials. The moiré potential is predicted to have a great impact on the interaction of light with the interlayer excitons. We discuss the observation of interlayer excitons in $MoSe_2/WSe_2$ heterobilayers performing μ-PL measurements. Due to the weaker coupling strength between the electron and hole in the spatially separated arrangement, the luminscence from the interlayer excitons is shifted around 200 nanometers. The interlayer excitonic resonance is further characterized by a distinct, non-trivial peak structure, which indicates the involvement of a moiré superpotential.

DS 4.8 Mon 11:45 POT 81

Interlayer excitons and band alignment in MoS_2/GaSe heterostructures. — •Christian Wagner[1,2], Mahfujur Rahaman[2], Dietrich R.T. Zahn[2], and Sibylle Gemming[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany

We study the influence of the $(GaSe)_n/(MoS_2)_m$ heterostack composition on the band alignment and the interlayer exciton energy using *ab initio* calculations.

The electronic interaction between individual layers in a 2D heterostack is often reasonably described by a perturbation of the physical effects of the isolated layers by additional electrostatic doping and screening. In terms of optical properties, however, the formation of bound interlayer excitons composed of electrons from one layer and holes from the neighboring layer is possible. These states are measured experimentally by photoluminescence and photocurrents, e.g. in the case of MoS_2 on GaSe due to its type-II band alignment [1].

The interlayer excitons can be approximately located in k-space and energy from density functional theory by relating the band structures of the heterostack to the band structure of the individual layers. This is allowed due to the weak hybridization of electronic states between the two materials. Furthermore, the many-body description allows extracting the exciton binding energies and oscillator strengths in order to obtain the respective spectral signatures.

[1] M. Rahaman *et al.*, J. Phys.: Condens. Matter **31**, 114001 (2019)

DS 4.9 Mon 12:00 POT 81

Biexcitons in 2D transition metal dichalcogenide from first principle: binding energies and fine structure — •Abderrezak Torche and Gabriel Bester — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, D-20146 Hamburg, Germany

Reducing the dimensionality of a system enhances quasiparticles interaction and leads to the formation of Coulomb bound complexes which govern most of the optical properties of semiconductors. Among these complexes, biexcitons are of special interest. Theoretically, first principle treatment of biexcitons, on the same theoretical footing as excitons and trions, is now possible thanks the the newly developed methodology of Ref. [1] which uses a hybrid approach combining configuration interaction and green function methods for the description of many-electrons many-holes excitations. This methodology is applied here to study the binding and fine structure of biexcitons in different transition metal dichalcogenides. The resulting binding energies agree better with experimental values a compared to previous effective mass treatment. The fine structure of biexcitons is shown to be highly dependent on temperature and become very dense (e.g. have many sub-peaks that are separated by hundreds of micro-eV to few meV) at room temperature.

[1] Torche, A., and Bester, G. (2019).PRB,100(20), 201403.

DS 4.10 Mon 12:15 POT 81

In-plane anisotropy of the photon-helicity induced linear Hall effect in few-layer WTe_2 — •Simon Steinhauser[1,2], Paul Seifert[1,2], Florian Sigger[1,2], Jonas Kiemle[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Christoph Kastl[1,2,4], Ursula Wurstbauer[1,2,5], and Alexander Holleitner[1,2] — [1]Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, D-85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstrasse 4, D-80799 München, Germany — [3]Advanced Materials Laboratory, Tsukuba, Ibaraki 305-0044, Japan — [4]Molecular Foundry, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley, California 94720, USA — [5]Institute of Physics, University of Münster, Wilhelm-Klemm-Strasse 10, D-48149 Münster, Germany

Using Hall photovoltage measurements, we demonstrate that a linear transverse Hall voltage can be induced in few-layer WTe_2 under circularly polarized illumination. We find that the photon-helicity induced Hall effect is strongly anisotropic with respect to the crystal axis. Our results are consistent with the Berry curvature and its dipolar distribution due to the breaking of inversion symmetry. We also studied how the Hall voltage changes with varying layer numbers. Time resolved optoelectronic autocorrelation spectroscopy shows the comparatively long spin lifetime of carriers caused by the momentum-indirect electron and hole pockets in WTe_2.

DS 4.11 Mon 12:30 POT 81

Characterization of interlayer excitons in $MoSe_2$-WSe_2 heterostructures in high magnetic fields — •Johannes Holler[1], Michael Kempf[3], Jonas Zipfel[1], Mariana Ballottin[2], Anatolie Mitioglu[2], Philipp Nagler[1], Michael Högen[1], Alexey Chernikov[1], Peter Christianen[2], Christian Schüller[1], and Tobias Korn[3] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]High Field Magnet Laboratory (HFML EMFL), Radboud University Nijmegen, Netherlands — [3]Institut für Physik, Universität Rostock, Germany

In the recent years, the research on transition-metal dichalchogenides (TMDCs) and especially their heterostructures has increased a lot. These heterostructures are fabricated by stacking two different TMDCs on top of each other. With the right material combination, a type-II band alignment can be achieved and electrons and holes are spatially separated forming so-called interlayer excitons (IEXs).

Here, we study these IEXs in $MoSe_2$-WSe_2 heterostructures. In low-temperature PL measurements in magnetic fields of up to 30T, we observe a giant valley-selective splitting and a resulting near-unity valley polarization. In time-resolved measurements, we track the buildup of IEX valley polarization in the magnetic field. We also find a clear dependence of the magnetic-field behavior of the IEX on the stacking angles.

DS 4.12 Mon 12:45 POT 81

Defect-related photoluminescence of WS_2 monolayers — •Marcel Ney, Aswin Asaithambi, Lukas Madauss, Marika Schleberger, Axel Lorke, and Günther Prinz — Faculty of Physics and CENIDE, University Duisburg-Essen, Germany

Two-dimensional transition metal dichalcogenide (TMD) monolayers interact efficiently with visible light due to the direct band gap nature at the K-point in momentum space. The result of the quantum confinement effects in two dimensions is a strong electron-hole Coulomb interaction, leading to a large exciton binding energy, which makes this material very promising for optoelectronic devices.

We will present low-temperature photoluminescence-spectroscopy (PL) measurements, which show the influence of laser-irradiation with different excitation powers on WS_2 monolayers grown on a standard Si/SiO_2 substrate via a chemical vapor deposition (CVD) process.

In the PL investigations, we observed a defect-related emission D_1, which can be assigned to adsorbate-decorated defect complexes [1]. The nature of this defect-related state investigated by laser-power-dependent measurements, will be presented in this contribution. During a laser excitation cycle, a laser-activated emission with a higher energy than the defect-related emission D_1, occurs. Furthermore, an-

other defect-related emission D_2 was observed. Due to the annealing properties after laser-irradiation we identify this emission as a mono-sulfur vacancy decorated with physisorbed adsorbates [2].

[1] Z. He et al., ACS Nano 10, 5847 (2016)
[2] V. Carozo et al., Science Advances 3, e1602813 (2017)