DS 3: 2D Materials 1 (joint session HL/CPP/DS)

Time: Monday 9:30–12:45 Location: H36

Invited Talk DS 3.1 Mon 9:30 H36

g-factors in van der Waals heterostructures: revealing signatures of interlayer coupling — •Paulo E. Faria Junior — University of Regensburg, Regensburg, Germany

The interplay of the spin and the orbital angular momenta of electrons in semiconductors governs the observed Zeeman splitting, often described by the effective g-factors. In the realm of 2D materials, transition metal dichalcogenides (TMDCs) are ideal candidates to explore the manifestation of coupled spin and orbital degrees of freedom under external magnetic fields. In this talk, I will cover the basic physics behind the Zeeman splitting and effective g-factors, emphasizing the recent first-principles developments in monolayer TMDCs that nicely reproduce the available experimental data. These new theoretical insights demystify the valley-Zeeman physics in TMDCs and finally establish a connection to the vast existing knowledge in the area of III-V materials. Beyond monolayers, I will discuss TMDC-based van der Waals heterostructures, particularly MoSe2/WSe2 and WS2/graphene systems, in which the spin-valley physics and g-factors encode valuable information about the interlayer coupling.

DS 3.2 Mon 10:00 H36

Optical Properties of Encapsulated Transition-Metal Dichalcogenide Monolayers, Bilayers, and Heterostructures — •Manan Shah[1], Philip Klement[1], Sangam Chatterjee[1], Kyungnam Kang[2], Eui-Hyeok Yang[2], and Arash Rahimi-Iman[1] — [1]I. Physikalisches Institut und Zentrum für Materialwissenschaften, Justus-Liebig Universität Gießen, D-35392, Germany — [2]Department of Mechanical Engineering, Stevens Institute of Technology, Hoboken, NJ, 07030, USA

Van-der-Waals heterostructures (vdW-HSs) based on 2D-layered materials have received unrivaled attention among nanomaterials due to their promising optoelectronic properties induced by moiré potential landscapes; secondly, their strong light-matter interactions; and third, the promise of bandgap engineering capabilities. The optical properties of transition-metal dichalcogenides (TMDs) depend considerably on the substrate, stacking configuration, interface quality, and encapsulation. As more and more layered materials have come into the focus, the demand for a comprehensive understanding of their optical, optoelectronic, and vibronic properties is increasing drastically.

We focus on the discussion of photoluminescence and the Raman response of tungsten-based TMD monolayers and stacks thereof [1, 2], as well as encapsulated configurations. We further aim at unraveling structural alterations and emission properties by monitoring the temporal behavior in their responses. [1] Semiconductors 2019, 53, 2140. [2] Sci. Rep. 2022, 12, 6939.

DS 3.3 Mon 10:15 H36

Electrically Tunable Photoluminescence in Monolayer MoS_2 and graphene/MoS_2 Heterostructures — •Tarlan Hamzayev and Giancarlo Soavi — Institute of Solid-State Physics, Friedrich Schiller University Jena, Germany

The optical response of monolayer (ML) transition metal dichalcogenides (TMDs) is dominated by the co-existence, even at room temperature, of excitons, bi-excitons, and trions.

The photoluminescence (PL) emission of these quasi-particles can be modulated via external knobs, such as doping, pressure and strain. In particular, the PL emission from the neutral exciton is greatly modulated during the crossover from the undoped to the highly doped regime [1]. In the latter case, PL emission is mainly suppressed due to the presence of trions, which have a fast non-radiative decay.

In this work, we study the gate dependence of the PL emission in encapsulated ML MoS_2 and ML graphene/MoS_2 heterostructures (HS). We show that in the HS region the PL emission mainly comes from neutral excitons even at large values of external gate voltage, thus confirming that graphene is an efficient filter for PL emission [2]. This work clarifies the interplay between charge transfer and PL filtering in graphene/TMD layered HS.

[1] Mak, K. F. et al. Nature materials 12, 207-211 (2013).

[2] Lorchat, E. et al. Nature Nanotechnology 15, 283-288 (2020).

15 min. break

DS 3.4 Mon 10:45 H36

Integration of Transferable Organic Semiconductor Nanosheets with 2D Materials for van der Waals Heterojunction Devices — •Sirri Batuhan Kalkan[1], Emad Najafidehaghani[2], Ziyang Gan[2], Fabian Alexander Christian Apfelbeck[1], Uwe Hübner[3], Antony George[2], Andrey Turchanin[2], and Bert Nickel[1] — [1]Faculty of Physics and CeNS, Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 Munich, Germany — [2]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University Jena, Lessingstr. 10, 07743, Jena, Germany — [3]Leibniz Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, 07745, Jena, Germany

Evaporation of organic semiconductors (OSC) on atomically thin transition metal dichalgonides (TMD) for van der Waals (vdW) heterojunctions is limited by obstructed growth of the organic small molecules on the TMD surface. For the realization of such vdW heterojunction devices, we have established a transfer technique that allows for wafer-scale fabrication of 50 nm OSC nanosheets on TMDs. A key feature of this transfer is the controlled release of the ultrathin OSC film from a water-soluble sacrificial film by a suited wetting geometry. We demonstrate functional and highly ordered OSC nanosheets on prefabricated electrodes and TMD monolayers. Devices fabricated this way include unipolar, ambipolar and anti-ambipolar field-effect transistors [1].

References: [1] Kalkan et al., Wafer scale synthesis of organic semiconductor nanosheets for van der Waals heterojunction devices, npj 2D Materials and Applications 5, 92 (2021)

DS 3.5 Mon 11:00 H36

Non-resonant and resonant low-frequency Raman scattering in twisted TMDC bilayers at millikelvin temperatures — •Hendrik Lambers[1], Nihit Saigal[1], Torsten Stiehm[1], Florian Sigger[2], Lukas Sigl[2], Mirco Troue[2], Johannes Figueiredo[2], Alexander Holleitner[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany

Twisted TMDC bilayers are subject of many current studies because they can host many body physics and correlated phases such as superconductors and Mott insulators.[1] The moiré potential evolving with a twist angle or lattice constant mismatch could also be exploited to simulate Mott-Hubbard physics. The interlayer coupling within the bilayer correlates with the interlayer breathing mode and the shear mode, which can be characterized by low frequency Raman spectroscopy.[2] We study TMDC heterobilayers of WSe2 and MoSe2 by resonant and non-resonant Raman spectroscopy at millikelvin temperatures. The shear mode is resonant with the exciton transitions in both monolayers and its lineshape and transition energy are modified due to coupling to the exciton continuum. In addition, several sharp and highly resonant modes are observed in the high frequency Raman spectrum. We acknowledge financial support via DFG WU 637/7-1 and SPP2244. [1] L. Sigl et al., Phys. Rev. Research 2, 042044(R) (2020) [2] J. Holler et al., Appl. Phys. Lett. 117, 013104 (2020)

DS 3.6 Mon 11:15 H36

Investigating Twist Angle Dependence of Exciton Resonances in WSe_2/$MoSe_2$ Heterostructures — •Chirag Palekar, Tobias Manthei, Bárbara Rosa, and Stephan Reitzenstein — Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany

Artificially produced TMDC heterostructures (HS) realized by stacking two different TMDC monolayers (ML) are a new class of promising semiconducting heterostructures. Due to their type-II band alignment, TMDC HSs tend to host the spatially indirect interlayer excitons (IX) where electrons and holes are located in conduction and valence bands, respectively, of the different layers. Here we study the twist angle dependence of IX resonances employing micro-photoluminescence excitation (PLE) measurements on twisted WSe_2/$MoSe_2$ heterobilayer. PLE measurements reveal anti-correlation between linewidth and emission energy of IX. Resonant excitation at intralayer exciton energies of constituent ML yields high emission intensity of the IX with linewidth narrowing above 10 meV. We measure a drastic reduction in PL emission from IX for twist angles in the range of 10°- 50° due to large inter-

layer separation. Moreover, we show a noticeable IX exciton resonance separation which increases as function of twist angle i.e. from 0° (67 meV) to 24° (96 meV) along with observable red shift in IX emission energy. This fundamental study of excitons resonances deepens the current understanding of physics of twisted TMDC heterostructures and paves the way for future experiments and theoretical work.

DS 3.7 Mon 11:30 H36

Counterintuitive electric-field dependence of weak antilocalization in a bilayer graphene/WSe_2 heterostructure — Julia Amann[1], Tobias Völkl[1], Tobias Rockinger[1], Denis Kochan[2], Kenji Watanabe[3], Takashi Taniguchi[3], Jaroslav Fabian[2], Dieter Weiss[1], and •Jonathan Eroms[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany — [2]Institute of Theoretical Physics, University of Regensburg, Regensburg, Germany — [3]National Institute for Materials Science, Tsukuba, Japan

Heterostructures of bilayer graphene (BLG) and transition metal dichalcogenides (TMDC) were recently proposed as a means of generating a gate-tunable, proximity-induced spin-orbit coupling (SOC) in graphene. Total SOC splitting of the band structure increases monotonically with the out-of-plane electric field, as confirmed by recent charge transport experiments. To elucidate the spin relaxation caused by SOC, weak antilocalization (WAL) experiments are frequently employed. Contrary to the naïve expectation of a monotonic increase of the WAL effect strength with electric field D, we observe a maximum of WAL visibility around $D = 0$. This counterintuitive behaviour originates in the intricate dependence of WAL in graphene on two different spin lifetimes τ_{sym} and τ_{asy}, which are due to spin relaxation caused by the valley-Zeeman and Rashba terms, respectively. Our calculations, based on modeling spin precession by an 8×8 Hamiltonian of BLG with one-sided TMDC show the same non-monotonic dependence on D as the experimental data.

15 min. break

DS 3.8 Mon 12:00 H36

Millikelvin Spectroscopy on Degenerate Exciton Ensembles in van der Waals Bilayers — •Nihit Saigal[1], Torsten Stiehm[1], Hendrik Lambers[1], Florian Sigger[2], Lukas Sigl[2], Mirco Troue[2], Johannes Figueiredo[2], Alexander Holleitner[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany

Homo- and hetero-bilayers of transition metal dichalcogenides host a rich variety of interlayer exciton (IX) species where the electrons and holes reside in different monolayers. [1] This leads to enhanced lifetimes of IXs and also imparts them with a permanent dipole moment. [1,2] Such IXs provide an ideal platform for exploring many body physics such as dipole-dipole interactions and Bose-Einstein condensation. [2] We have investigated IXs in a heterobilayer of MoSe2 and WSe2 encapsulated in hBN, using temperature, laser power and time dependent photoluminescence (PL) spectroscopy down to millikelvin temperatures. At lowest temperatures and exciton densities, we observe a single low energy peak in the IX PL spectrum which has been attributed to be a signature of degenerate exciton gas. [2] We observe an unexpected nearly excitation power-independent IX energies at lowest temperatures (10 mK to ~10K) that converts into the well-known dipolar blue-shift at elevated temperatures. We acknowledge financial support by DFG via WU 637/4-2 and No. HO 3324/9-2 and SPP2244.

[1] B. Miller et al., Nano Lett. 17, 5229 (2017). [2] L. Sigl et al., Phys. Rev. Research 2, 042044 (R) (2020).

DS 3.9 Mon 12:15 H36

Infrared photocurrent in transition-metal dichalcogenide heterostructures — Jeong Woo Han[1], Peize Han[2], Yijing Liu[2], Paola Barbara[2], Thomas E. Murphy[3], and •Martin Mittendorff[1] — [1]Universität Duisburg-Essen, Fakultät für Physik, 47057 Duisburg, Germany — [2]Georgetown University, Department of Physics, Washington, 20057 DC, USA — [3]University of Maryland, Institute for Research in Electronics and Applied Physics, College Park, 20740 MD, USA

Heterostructures of transition metal dichalcogenites (TMDCs) have characteristic optical properties like the interlayer excitons due to the band offset between two adjacent TMDC layers. Such heterostructures are promising candidates for photodetectors with higher efficiencies compared to a single TMDC layer, furthermore, the interlayer excitation enables photocurrents at photon energies below the direct bandgap of each of the layers. Here we present measurements on a MoS_2/WS_2 heterostructure at photon energies of around 800 meV, which is significantly below the interlayer exciton. The cross-shaped structure of our samples allows measurements of the heterostructure as well as each individual layer. While at high photon energies photocurrents are observed in each of the layers, the low photon energy only leads to a photocurrent when the heterostructure is illuminated. We interpret this effect to be caused by intraband absorption and subsequent interlayer tunneling.

DS 3.10 Mon 12:30 H36

Strong exciton-plasmon coupling in hybrids of 2D semiconductors and metal supercrystals — •Lara Greten, Robert Salzwedel, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Monolayers of transition metal dichalcogenides (TMDC) are direct semiconductors that exhibit tightly bound excitons with uniquely large optical amplitudes. Thus, they are promising for optoelectronic applications and a prime example to investigate excitonic effects.

Complementary, plasmonic supercrystals, that are arrays of metal nanoparticles, support collective plasmon modes. They facilitate an impressive amplification of the electric near-field which allows to tailor electric fields on the nano-scale.

In the presented work, we theoretically consider exciton-plasmon coupling in a hybrid structure of a TMDC layer interacting with a single metal nano-particle or a two-dimensional supercrystal. For this purpose, we develop a Maxwell-Bloch theory where the excitons are described within the Heisenberg equation of motion framework and the metal nano-particles are treated as coupled dipoles in Mie theory.

Our studies reveal new "plexcitonic" eigenstates of the hybrid system. Furthermore, we are able to compute the scattered light in the near- and far-field explicitly and identify signatures of strong exciton-plasmon coupling featuring a Rabi splitting of tens of meV.