HL 8: 2D Materials II (joint session HL/CPP)

Time: Monday 15:00–18:15 Location: POT 81

HL 8.1 Mon 15:00 POT 81

Twist- and gate-tunable valley splitting in TMDC/CrI_3 heterostructures — •Klaus Zollner, Paulo E. Faria Junior, and Jaroslav Fabian — Institute of Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany

Van der Waals heterostructures composed of twisted monolayers promise great tunability of electronic, optical, and magnetic properties. Twistronics has already demonstrated its potential in tuning proximity spin-orbit and exchange coupling in graphene-based heterostructures [1,2]. In this talk, we present the strong manipulation of the valley splitting upon twisting and gating in TMDC/CrI_3 heterostructures [3]. In particular, upon twisting from 0° to 30°, the proximity-induced TMDC valence band edge exchange splitting can be reversed (−2 to 2 meV), while the TMDC conduction band edge exchange splitting remains nearly constant (−3 meV). Further giant tunability (few meV) of the proximity exchange coupling is provided by a transverse electric field. Consequently, twisting and gating then allow to tailor the valley splitting of the first intralayer exciton peak in the range of 0 to 12 meV in WSe_2/CrI_3, which is equivalent to gigantic external magnetic fields of up to about 60 Tesla.

This work was supported by DFG SFB 1277, DFG SPP 2244, and the EU Horizon 2020 Research and Innovation Program (Graphene Flagship).

[1] K. Zollner and J. Fabian, Phys. Rev. Lett. 128, 106401 (2022).
[2] Lee *et al.*, Phys. Rev. B 106, 165420 (2022).
[3] K. Zollner, P. E. F. Junior, J. Fabian, arXiv:2210.13794 (2022).

HL 8.2 Mon 15:15 POT 81

Giant Enhancement of Interlayer Exciton Luminescence in $WSe_2/WSe_2/MoSe_2$ in Heterotrilayers. — •Chirag Palekar, Ching-Wen Shih, Imad Limame, Bárbara Rosa, and Stephan Reitzenstein — Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany

TMDC heterolayers have gained lot on interest as a promising platform to study intricate many-body physics phenomena. Here we observe giant enhancement of interlayer exciton PL in a $WSe_2/WSe_2/MoSe_2$ heterotrilayers (HTL) system prepared by employing exfoliation and dry transfer method. The IX exciton forming at the heterojuction in the HTL region exhibits 10-fold increase in PL yield when compared to HBL region on the same sample. Such an enhancement can be attributed to the close to 0^0 twist angle between stacked WSe_2 homobilayers providing smaller interlayer separation and hybridization in the WSe_2 band structure, which in turn results in an efficient charge transfer. Further, PLE and reflection contrast reveal the twist angle dependence of the enhancement factor in such type II HTL systems as the large twist angel between WSe_2 homobilayers (57^0) results in only up to 10% percent enhancement of IX PL in the HTL region when compared with the HBL. This fundamental study of excitons in the HTL system deepens the current understanding of physics of twisted TMDC heterostructures and paves the way for future experiments and theoretical work.

HL 8.3 Mon 15:30 POT 81

Photoluminescence tuning in hybrid devices of monolayer transition metal dichalcogenides and rylene dyes — •Theresa Kuechle[1], Gergely Knorr[2], Kalina Peneva[2], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich Schiller University Jena, Lessingstraße 8, 07743 Jena, Germany

Monolayer transition metal dichalcogenides (TMDs) are direct gap semiconductors that hold great promise for applications in nanoscale photonics and optoelectronic devices. A viable path for the development of devices with advanced functionalities and tunable properties is the integration with other nanoscale systems such as nanowires [1] and molecules [2]. Here, we realize hybrid devices based on TMDs and rylene dyes and study their optical properties via steady state photoluminescence. Preliminary results show that the PL emission in hybrid structures of WS_2/CN_4PMI can be quenched by a factor of 3, in the case of WSe_2/CN_4PMI by 300. We tentatively assign this variation to a different band alignment in the two heterostructures and to the interplay between charge transfer (in type II) and energy transfer (in type I). Future experiments including ultrafast pump-probe spectroscopy of pristine and hybrid systems as well as hybridization of different (tunable) molecules will further elucidate the role of band alignment in the ultrafast charge and energy transfer processes at the nanoscale.

[1] Kim *et al.*, *ACS Nano* **14**, 9, 4323 (2020)
[2] Park *et al.*, *Adv. Mat. Interfaces* **8**, 12, 2100215 (2021)

HL 8.4 Mon 15:45 POT 81

Coherence of interlayer exciton ensembles in $MoSe_2/WSe_2$ heterobilayers — •Christos Paspalides[1], Mirco Troue[1], Johannes Figueiredo[1], Lukas Sigl[1], Manuel Katzer[2], Malte Selig[2], Andreas Knorr[2], Ursula Wurstbauer[3], and Alexander Holleitner[1] — [1]TU Munich — [2]Technische Universität Berlin — [3]University of Münster

Transition metal dichalcogenides exhibit strong light-matter interactions, which suggests them to be ideal candidates for novel 2D optoelectronic applications. Corresponding van der Waals heterostacks allow the excitation and formation of long-lived interlayer excitons [1]. We present coherence measurements of the ground state in such interlayer exciton ensembles by performing Michelson-Morley interferometry over a wide range of exciton density and temperature [2]. Moreover, we discuss the expansion dynamics of the interlayer excitons presumably driven by dipole-dipole interactions. The presented work paves the way towards a detailed understanding of excitonic many-body quantum phenomena in two-dimensional materials [3].

[1] B. Miller et al., Nano Letters 17, 5229 (2017).
[2] M. Troue and J. Figueiredo, et al (2023).
[3] L. Sigl et al., Signatures of a degenerate many-body state of interlayer excitons in a van der Waals heterostack, Phys. Rev. Res. 2, 042044 (2020).

15 min. break

HL 8.5 Mon 16:15 POT 81

Theoretical description of interlayer excitons in TMD homobilayers — •Ruven Hübner[1], Alexander Steinhoff[1], and Matthias Florian[2] — [1]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — [2]University of Michigan, Dept. of Electrical Engineering and Computer Science, Ann Arbor, MI, USA

In recent years, interlayer excitons in bilayers of transition metal dichalcogenides (TMDs) have received a rapid increase in attention. On the one hand, they feature the main characteristics of conventional excitons in the corresponding monolayers, namely an absorption spectrum in the optical regime combined with a high binding energy. On the other hand, they differ to such intralayer excitons by a massively increased life time, a non-zero dipole moment in the out-of-plane direction and a strong sensitivity to material combination as well as stacking arrangement of adjacent monolayers. In this talk we focus on special excitonic properties inside TMD homobilayers that are particularly demanding from a theoretical point of view. In this context we discuss moiré excitons in twisted bilayers as well as high-lying excitons and trions at around twice the band gap energy arising within a highly non-parabolic band dispersion.

HL 8.6 Mon 16:30 POT 81

Raman signature of interlayer coupling and lattice dynamics in 2D TMDCs — •Yang Pan[1,2] and Dietrich R. T. Zahn[1,2] — [1]Semiconductor Physics, Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Center for Materials, Architectures, and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany

Vertical stacking of two-dimensional (2D) homo- and heterostructures are intriguing research objects, as they are essential for fundamental studies and a key towards 2D device applications. It is paramount to understand the interlayer coupling in 2D materials and to find a fast yet precise characteristic signature. In this work, we report on a Raman fingerprint of interlayer coupling in 2D transition metal dichalcogenides (TMDCs). We observed that the out-of-plane B_{2g} vibrational mode is absent when two monolayers form a vertical stack yet remain uncoupled but emerges after strong coupling. Using systematic Raman, photoluminescence (PL), and atomic force microscopy (AFM) studies of WSe_2/WSe_2 homo-bilayers and $MoSe_2/WSe_2$ hetero-bilayers, we

conclude that the B_{2g} vibrational mode is a distinct Raman fingerprint of interlayer coupling in 2D TMDCs. Our further investigations confirmed its applicability on twisted 2D homo- and hetero-bilayers. Our results propose an easy, fast, precise, and reliable measure to evaluate the interlayer coupling and twisting angles in 2D TMDCs.

HL 8.7 Mon 16:45 POT 81

Correlated states of moiré interlayer excitons in twisted transition metal dichalcogenide heterostructures — •Nils-Erik Schütte[1], Niclas Götting[1,2], Frederik Lohof[1,2], and Christopher Gies[1,2] — [1]Institute for Theoretical Physics, University of Bremen, Bremen — [2]Bremen Center for Computational Material Science, University of Bremen, Bremen

Stacking two transition metal dichalcogenide (TMD) monolayers on top of each other with a small relative twist yields a moiré pattern with a long lattice period. Quasiparticles perceive the resulting bandstructure modulation as a potential landscape, making it possible to consider moiré heterostructures as a realization of a Bose-Hubbard model in a semiconductor material.

We address the question in how far correlated states of moiré excitons can emerge and study their phase transition behavior in relation to the twist angle between both monolayers. Expanding on previous results [1], we discuss the effect of nearest-neighbor interaction that gives rise to a variety of different phases, such as inhomogeneous insulating and supersolid phases. Special attention is paid to the possibility of local atomic reconstructions that are now known to occur at small twist angles.

[1] Götting et al., Phys. Rev. B 105, 165419 (2022)

HL 8.8 Mon 17:00 POT 81

Electronic structures of twisted bilayer graphene and tungsten diselenide investigated by transferable tight-binding-models — •Xiaoyu Liu, Stefan Blügel, and Hyun-Jung Kim — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Since the discovery of intrinsic unconventional superconductivity in the Moiré superlattice from bilayer graphene stacked with a small twist angle, a new venue so-called twistronics has opened. Beyond graphene, transition metal dichalcogenides as a class of two-dimensional (2D) materials have attracted much attention due to their interesting optical properties. With the growing interest in 2D layered materials, accurate models describing the band structure and electronic properties of twisted bilayer graphene and tungsten diselenide are highly desirable. Here, we provide sets of parameters for the transferable tight-binding (TB) model, based on the Slater-Koster (SK) scheme with the exponential scaling law for the interlayer and overlap integral parameters. The workflow, to obtain transferable TB model parameters, is automatized by introducing global optimization methods such as particle swarm optimization (PSO) and conformational space annealing (CSA) methods. The fitness of the parameter set is assessed not only by comparing with ab-initio band energies, but also with its orbital similarity. Accurately produced electronic structures of twisted bilayers graphene and tungsten diselenide provide a chance to research their unique electronic and optical attributes.

Hyun-Jung Kim acknowledges support by the AvH Foundation.

15 min. break

Invited Talk HL 8.9 Mon 17:30 POT 81

Time-resolved optical spectroscopy of 3R-stacked MoS_2 — •Swarup Deb, Michael Kempf, Rico Schwartz, and Tobias Korn — Institute of Physics, Rostock University

Manipulation of in-plane rotational and out-of-plane stacking symmetry in engineered two-dimensional (2D) crystals has provided means to realize a variety of exotic phases in extremely thin structures. The emergence of out-of-plane ferroelectricity in rhombohedrally-stacked 2D materials, such as boron nitride and transition metal dichalcogenides (TMDs), is a recent addition to this, but so far, most research on rhombohedrally stacked (3R) TMDs focussed on bilayer units.

Here, we present a systematic study of low-temperature absorption, differential reflectivity, and Kerr rotation in 3R-stacked MoS_2 as a function of thickness, aiming to probe the effects of ferroelectricity and interlayer charge transfer on ground-state exciton properties, valley and photocarrier dynamics. We observe clear signatures of an energetic splitting of the A exciton, as well as valley and energy relaxation dynamics on a few-ps timescale.

HL 8.10 Mon 18:00 POT 81

Constructing minimal tight-binding models for twisted TMDC bilayers — •Michael Winter, Dominik Benner, and Tim Wehling — I. Institute of Theoretical Physics, Universität Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany

Transition metal dichalcogenides bilayers attract considerable attention within the last years due to the wide range of observable correlation effects, e.g. superconductivity, exciton condensation and therelike. One possible parameter to tune these phenomena is the twist angle between the two layers.

We study the electronic structure of twisted transition metal dichalcogenides from ab initio DFT calculations and subsequent Wannier construction on untwisted snapshots of commensurate structures. By choosing a subspace of only three Wannier orbitals per transition metal, we construct a minimal model for the description of twisted bilayers.