Mid-term Report Colloquium

March 21 to March 23, 2022

Penck Hotel, Dresden

Book of Abstracts

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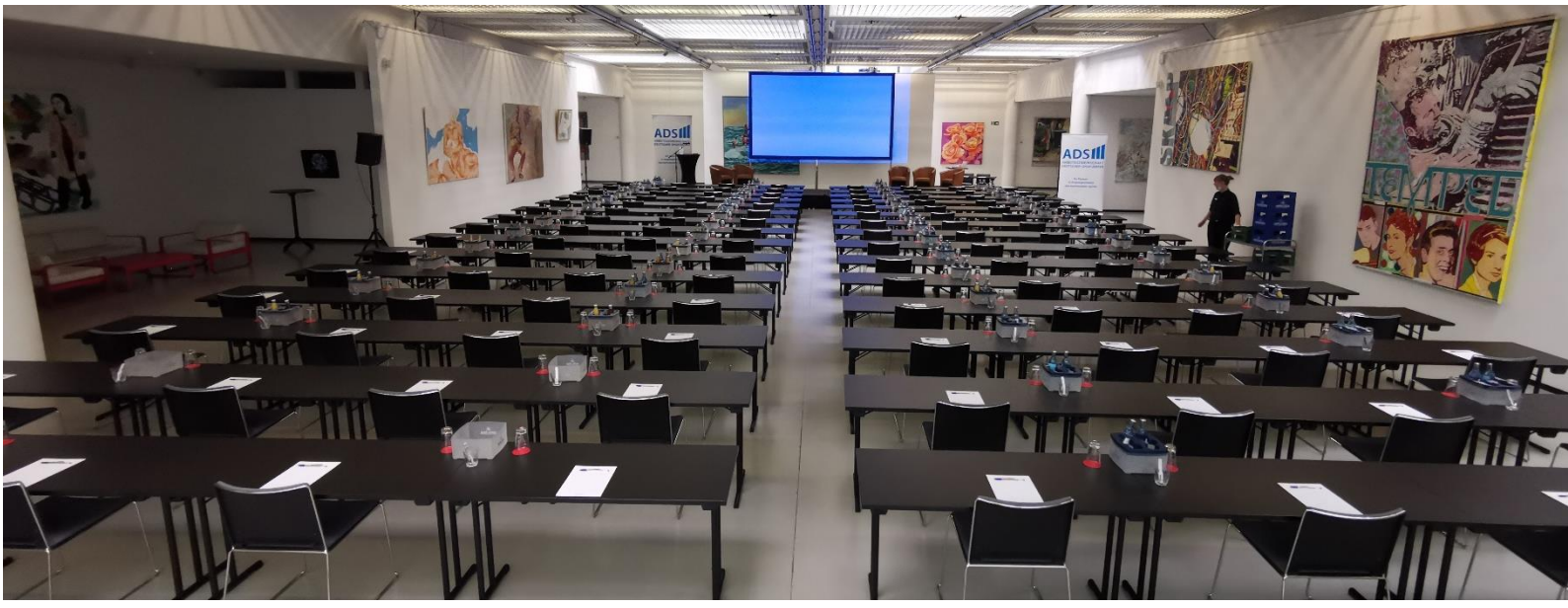
Poster Session 2 (Wed, 11:30 – 13:15): nr. 18 – 38



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Nr. 01: Tuning and mapping hybrid polaritons at the nanoscale

Elyas Khairi, Hannah C Nerl and Katja Höflich

In two-dimensional (2D) materials light-matter interaction can be significantly enhanced by polaritons. A polariton is a quasiparticle that results from coupling between an electromagnetic wave, such as light, and a dipole carrying excitation in matter. Typical matter excitations are collective oscillations of free electrons (surface plasmon polaritons), lattice vibrations (phonon polaritons) or due to electrons lifted from the valence to the conduction band (exciton polaritons). Stacking of different 2D materials can lead to coupling of polaritons to produce hybrid modes with a large degree of tunability in the type of excitation, their coupling strength, and their localization and propagation behaviour.

Our project is focused on studying the optical properties arising from interlayer interactions in 2D heterostructures with the goal of realizing hybrid polaritonic modes with nanoscale confinement and low losses. Graphene and single crystalline silver in combination with hexagonal boron nitride (hBN) are first produced and then structured on the nanoscale with focused He ion beams. Initially, each material system is patterned and studied separately to evaluate the effects of the He ion beam to optimize the patterning parameters. The materials individually and in combination are then studied using electron energy-loss spectroscopy (EELS) in a scanning transmission electron microscope (STEM). The polaritonic modes arising are then mapped at the nanoscale.

Nr. 02: Light-matter coupling of Moiré Excitons in Twisted TMDC Hetero-structures

S. Reitzenstein, C. Schneider, and C. Gies

Our consortium investigates the physics of light-matter coupling of excitons in twisted TMDC heterobilayers (HBLs), including their coupling to optical cavity modes. A central focus of the project lies on collective phenomena in such structures, including Bosonic Condensation, superradiant emission, and Bose Hubbard physics of excitons.

The contribution summarizes our efforts and progress towards these highly ambitious goals:

- In slightly twisted MoSe2/WSe2 heterostructures, we found peculiar emission features exhibiting an intrinsic circular polarization degree arising from a dynamical relaxation [1]. The intriguing feature is now studied in detail as function of the Moiré twist angle.
- First generation of cavities with embedded heterostructures display pronounced luminescence features, and are highly promising towards the observation of strong light-matter coupling in van-der-Waals Heterostructures.
- Moiré hetero-bilayers with different twist angles are studied by time-resolved photoluminescence and photon autocorrelation to identify signatures of superradiance.
- First theoretical results investigate the possibility of a phase transition between Mott and superfluid phases in moiré heterostructures and lay the foundation for material-specific calculations of the key parameters U and t of the Bose-Hubbard model [2].
- A SPP-internal topical review article addresses approaches and challenges in modeling the many-body optical properties of van der Waals materials [3].

References:

[1] J. Michl et al., arXiv:2105.09948 (2021)
[2] N. Götting, F. Lohof and C. Gies, arXiv:2201.10877 (2022)
[3] C. Gies and A. Steinhoff, Laser & Photonics Reviews 2021, 2000482 (2021), DOI: 10.1002/lpor.202000482

Nr. 03: Characterization of Moiré Excitons in Twisted TMDC Hetero-structures for Investigation of Collective Emission Effects

C. C. Palekar, M. von Helversen, B. Rosa, C. Schneider, C. Gies and S. Reitzenstein

Twisted TMDC heterobilayers (HBLs) fabricated by systematically stacking monolayers (MLs), host interlayer excitons with strong permanent dipole moment. These interlayer excitons (IX) experience tight spatial trapping due to the Moiré potential which is result of lattice mismatch or rotational misalignment. Consequently, the system can be approximated by a perfectly ordered array of two-level emitters [1], where the density of emitters is varied by the heterobilayers' twist angle within a supercell. This unique material system is inherently an ideal playground for exploring the foundations of Dicke superradiance [2] of coupled photon emitters and to provide means of tunability that can only be dreamt of in monolithic semiconductor nanostructures.

Here, we discuss our results towards the preparation and characterization of localized emitters which resides in TMDC HBL. We start with the sample preparation by stacking mechanically exfoliated MLs of $MoSe_2$ and WSe_2 on a distributed Bragg reflector (DBR) substrate. Subsequently we determine the twist angle by comparing the angle-resolved SHG signal from individual MLs. Further, low temperature photoluminescence measurements show the emission from localized interlayer excitons in the twisted TMDC HBLs. The reduced lifetime of interlayer exciton at higher energies indicate presence of spatial localized emitters as demonstrated in previous studies [3]. Additionally, we investigate intrinsic circularly-polarized Moiré exciton emission in a twisted HBL [4]. Finally, we plan to incorporate pre-characterized TMDC HBLs into the dielectric DBR cavities which will provide a platform to understand the collective emission effects as well as Bose-Einstein condensation of Moiré exciton-polaritons.

References:

[1] H. Yu, G. Bin Liu, J. Tang, X. Xu, and W. Yao,Sci. Adv., vol. 3, no. 11, 2017.
[2] R. H. Dicke, Phy. Rev., vol. 93, no. 1, 1954.
[3] J. Choi et al., Phys. Rev. Lett., vol. 126, no. 4, p. 047401, Jan. 2021.
[4] J. Michel et al., arXiv:2105.09948 (2021)

Nr. 04: Magnetic Skyrmion in a 2D Ferromagnet from a Defect Driven Dzyaloshinskii–Moriya Interaction

Anirban Chakraborty, Stuart Parkin

Recently, two-dimensional (2D) ferromagnets have gained much attention for hosting magnetic skyrmions, a nano-scopic spin texture with chiral boundaries. Of particular interest is the ferromagnetic, metallic Fe_3GeTe_2 (FGT), which has a comparatively high Curie temperature (150–220 K). In addition, since FGT is metallic and, therefore, it offers the possibility of the manipulation of spin textures via spin currents. The crystal is presumed to have a centrosymmetric structure, and yet literature reports on the observation of chiral Néel skyrmions in this compound. This incites interest on the origin of the Dzyaloshinskii–Moriya vector exchange interaction (DMI) that stabilizes such chiral nano-objects in this material. Here, in this talk, the observation of Néel type skyrmions in single crystals of FGT via Lorentz transmission electron microscopy (LTEM) will be discussed. With the help of detailed X-ray diffraction structure analysis it will be shown that FGT lacks an inversion symmetry as a result of an asymmetric distribution of Fe vacancies. This vacancy-induced breaking of the inversion symmetry of this compound is a surprising and yet, a novel observation and is a prerequisite for a DMI which accounts for the chiral Néel skyrmion phase. This phenomenon is likely to be common to many 2D van der Waals (vdW) materials and suggests a path to the preparation of many such acentric compounds. Furthermore, it has also been found that the skyrmion size in FGT is strongly dependent on its thickness: the skyrmion size increases from ~100 to ~750 nm as the thickness of the lamella is increased from ~90 nm to ~2 µm. This extreme size tunability is a feature common to many low symmetry ferro- and ferri-magnetic compounds.

Nr. 05: Modelling TMDC/2D perovskite heterostructures for charge and energy transfer

Agnieszka Kuc

Van der Waals heterostructures are currently the focus of intense investigation; this is essentially due to the unprecedented flexibility offered by the total relaxation of lattice matching requirements and their new and exotic properties compared to the individual layers. Here, we investigated the hybrid transition-metal dichalcogenide (TMDC)/2D perovskite heterostructures, such as WS_2/$(PEA)_2PbI_4$ (where PEA stands for phenylethylammonium), but also other. We present the first density functional theory (DFT) calculations of a heterostructure ensemble, which revealed a novel band alignment, where direct electron transfer is blocked by the organic spacer of the 2D perovskite. In contrast, the valence band forms a cascade from TMDC through the PEA to the PbI_4 layer allowing hole transfer. These predictions are supported by optical spectroscopy studies, which provide compelling evidence for both charge transfer and nonradiative transfer of the excitation (energy transfer) between the layers. Our results show that TMDC/2D perovskite heterostructures provide a flexible and convenient way to engineer the band alignment

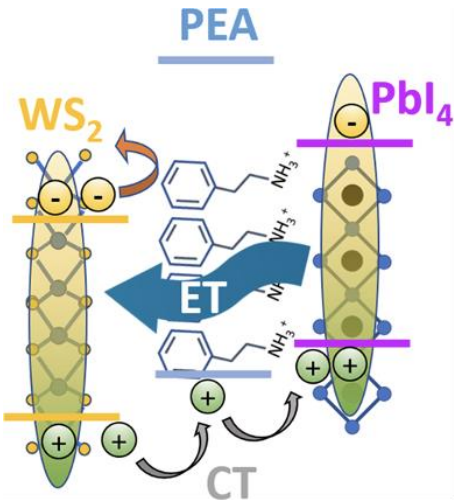


Figure: Summary of the band alignment in the PEPI/WS_2 heterostructure resulting from DFT calculations. The charge transfer(CT) and energy transfer (ET) paths are indicated

References:

Nonradiative Energy Transfer and Selective Charge Transfer in a WS2/(PEA)2PbI4 Heterostructure
Miriam Karpińska, Minpeng Liang, Roman Kempt, Kati Finzel, Machteld Kamminga, Mateusz Dyksik, Nan Zhang, Catherine Knodlseder, Duncan K. Maude, Michał Baranowski, Łukasz Kłopotowski, Jianting Ye, Agnieszka Kuc, and Paulina Plochocka
https://doi.org/10.1021/acsami.1c08377

Nr. 06: Relaxation and the Moiré Potential for Homobilayers of TMDCs

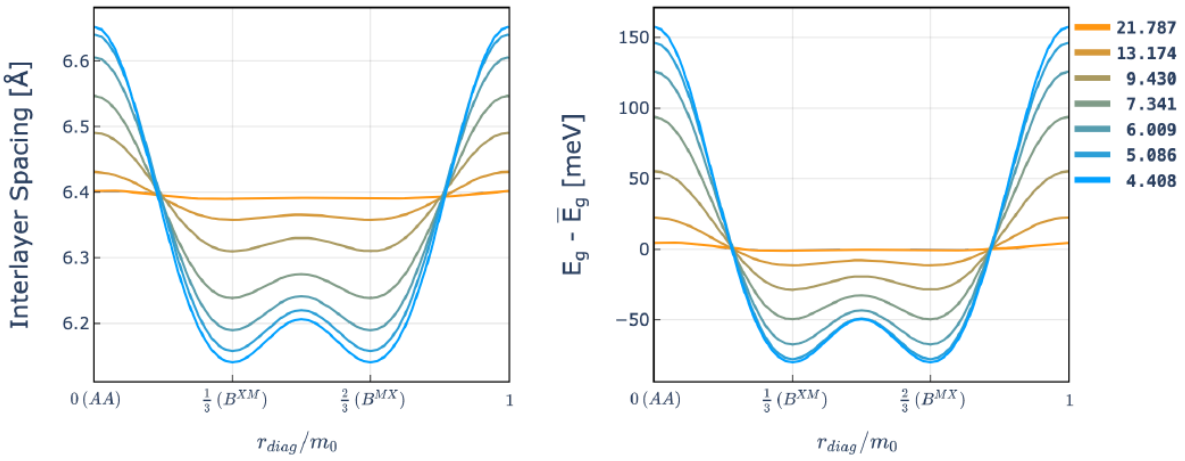
Carl Emil Mørch Nielsen, Miguel da Cruz, Abderrezak Torche and Gabriel Bester

In recent years, the research of transition metal dichalcogenides has amassed much attention due to its interesting properties. The two-dimensional structure of TMDs allows for strong localisation of excited states resulting in high binding energies. Much is already known about the properties of mono-, bilayer and bulk TMDs, and so, another interesting thing to explore is the field of twistronics. The theoretical ab-initio approach shows an immediate challenge to overcome; large systems, where the moire unit cell may hold millions of atoms.

In this project, the aim is to theoretically study Moiré confined optical excitations in twisted TMD vdW-homo and heterostructures. This includes excitons, trions, biexcitons and higher terms. Both spatially direct and indirect types of excitations will be investigated.

Regarding the progress of this project, we have successfully integrated a force-field based method of relaxation using LAMMPS as suggested in a paper by Jain et. al [ref]. We have re-parameterized the SW and KC potentials seen in this paper to better fit the bandgap, which is the foundation of accurately modeling the moire potential. Moreover, we have expanded the model to also include TMDs with telluride in the chalcogen sites. Furthermore, we are slowly expanding it to also include heterostructured bilayers.

Generally, we find that the moire potential varies on a scale that requires very accurate modeling of the lattice corrugation, since this will be the main contributor to this variation.



We also show that in case of large moire structures, e.g. angles below about two degrees, the lattice corrugation can be quite accurately depicted by continuum-like models.

The next steps for us, which we are already slowly taking, are then to investigate the excited state properties with our group-developed code.

Nr. 07: Signatures of superconducting proximity effects in two-dimensional (2D) superconductor/ferromagnet bilayers with a helimagnetic metal

Alfredo Spuri, Angelo Di Bernardo

Several studies [1][2] performed on three-dimensional (3D) superconductor/ferromagnet (S/F) structures have shown that a viable route to generate fully spin-polarized (i.e., spin-triplet) superconducting states consists in using F materials with an intrinsically inhomogeneous magnetization [3].

The metallic F $Cr_{1/3}NbS_2$ shows a magnetically inhomogeneous ground state, where the magnetization follows a helimagnetic pattern along the crystallographic c-axis. Previous reports on 2D flakes of $Cr_{1/3}NbS_2$ have also shown that the helimagnetic spin texture in this material can be modulated via soliton excitations [4] activated by an in-plane applied magnetic field H.

We have fabricated 2D S/F bilayers consisting of $Cr_{1/3}NbS_2$ stacked via van der Waals interactions onto NbS_2 (2D S) and we have characterized their low-temperature magnetotransport properties to find evidence for spin-triplet states. Our results demonstrate strong evidence for a superconducting proximity effect occurring in the $Cr_{1/3}NbS_2/NbS_2$ system which manifests through the emergence of H-tunable reentrant resistive states below the superconducting transition of the bilayers and through a non-monotonic variation of the superconducting critical temperature (Tc) with the applied H. The latter result is possibly consistent with the generation of long-ranged spin-triplet pairs at the $NbS_2/Cr_{1/3}NbS_2$ interface.

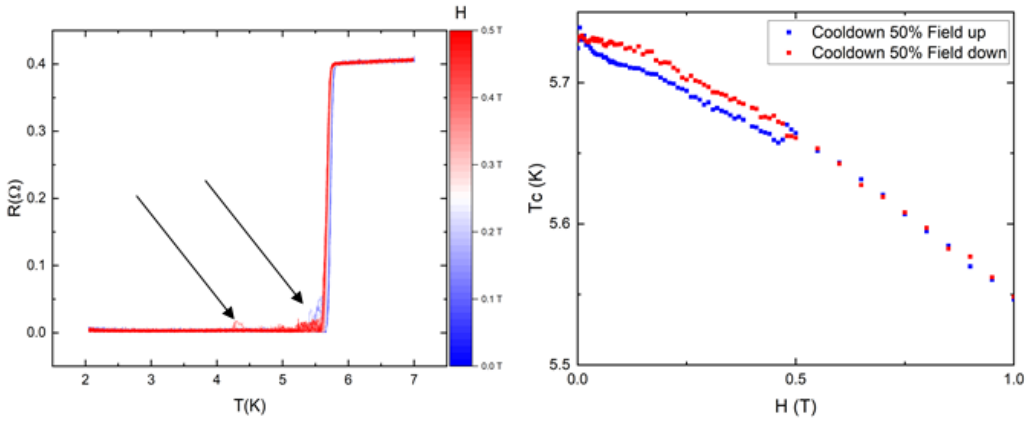


Figure 1: R(T) measurements (left) and extracted critical temperature (Right) at different magnetic fields for a $Cr_{1/3}NbS_2/NbS_2$ bilayer.

References:

[1] JWA Robinson, JDS Witt, MG Blamire, Controlled injection of spin-triplet supercurrents into a strong ferromagnetScience 329 (5987), 59-61.

[2] Di Bernardo, A., Diesch, S., Gu, Y. et al., Signature of magnetic-dependent gapless odd frequency states at superconductor/ferromagnet interfaces. Nat Commun 6, 8053 (2015).

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[4] Wang, L., Chepiga, N., Ki, D.-K., Li, L., Li, F., Zhu, W., Kato, Y., Ovchinnikova, O. S., Mila, F., Martin, I. et al., Controlling the Topological Sector of Magnetic Solitons in Exfoliated Cr1/3NbS2 Crystals, Phys. Rev. Lett. 118, 257203 (2017)

Nr. 08: Towards two-dimensional superconducting spintronics: 'Mirage'-gap, Josephson effect, and triplet superconductivity in Ising superconductors

Sourabh Patil, Alfredo Spuri, Wolfgang Belzig, Elke Scheer, Angelo Di Bernardo, Gaomin Tang, Christoph Bruder,Raffael Klees, Sourabh Singh, Maya Klang, Hen Alpern, Oded Millo, Hadar Steinberg

Superconductivity is commonly destroyed by a magnetic field due to orbital or Zeeman-induced pair breaking. Surprisingly, the spin-valley locking in a two-dimensional superconductor with spin-orbit interaction makes the superconducting state resilient to large magnetic fields. We investigate the spectral properties of such an Ising superconductor in a magnetic field considering disorder [1]. The interplay of the in-plane magnetic field and the Ising spin-orbit coupling leads to noncollinear effective fields. We find that the emerging singlet and triplet pairing correlations manifest themselves in the occurrence of "mirage" gaps: at (high) energies of the order of the spin-orbit coupling strength, a gaplike structure in the spectrum emerges that mirrors the main superconducting gap. We show that these mirage gaps are signatures of the equal-spin triplet finite-energy pairing correlations and due to their odd parity are sensitive to intervalley scattering.

An in-plane magnetic field applied to an Ising superconductor converts spin-singlet Cooper pairs to spin-triplet ones. In [2], we study a Josephson junction formed by two Ising superconductors that are proximitized by ferromagnetic (FM) layers. This leads to highly tunable spin-triplet pairing correlations which allow to modulate the charge and spin supercurrents through the in-plane magnetic exchange fields. For a junction with a nonmagnetic barrier, the charge current is switchable by changing the relative alignment of the in-plane exchange fields, and a π state can be realized. Furthermore, the charge and spin current-phase relations display a φ0-junction behavior for a strongly spin-polarized FM barrier.

The presence of a triplet pairing channel quantitatively changes the superconducting state and, hence, the spectral properties. We present preliminary studies of the influence of a triplet order parameter on the mirage gap.

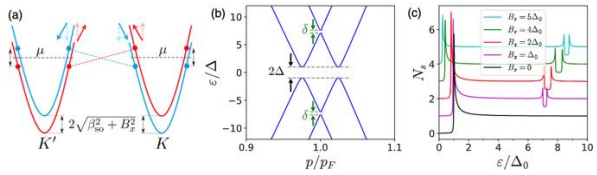

Figure 1: In-plane magnetic field induced mirage gap at an energy $\approx \beta_{so} = 7$.

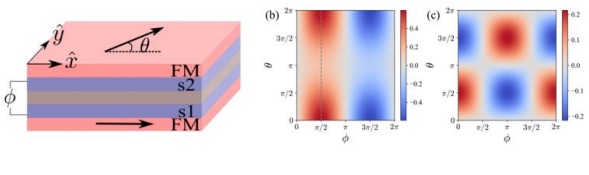

Figure 2: An Ising Josephson junction (a). Charge and spin supercurrents (b,c).

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[1] G. Tang, C. Bruder, and W. Belzig, Magnetic Field-Induced "Mirage" Gap in an Ising Superconductor, Phys. Rev. Lett. 126, 237001 (2021).

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Nr. 09: Towards two-dimensional (2D) superconducting spintronics: Fabrication, tunneling spectroscopy and magnetotransport of 2D superconductor/ferromagnet systems

Sourabh Singh, Maya Klang, Pradheesh Ramachandran, Hen Alpern, Oded Millo, Hadar Steinberg, Gaomin Tang, Christoph Bruder, Raffael Klees, Alfredo Spuri, Sourabh Patil, Wolfgang Belzig, Elke Scheer, Angelo Di Bernardo

The interplay between ferromagnetism and superconductivity has been intensively explored in systems and devices based on three-dimensional (3D) superconductor/ferromagnet (S/F) heterostructures. These studies [1-4] have also contributed to establish the conditions under which fully spin-polarized (spin-triplet) Cooper pairs can be generated in 3D S/F heterostructures – which has been key for the development of the field of superconducting spintronics [1].

With the aim of novel superconducting spintronic devices based on 2D van der Waals (vdW) materials, we have carried out a systematic optimization of the fabrication of 2D vdW S/F systems and characterized the spectroscopic and magnetotransport properties of the as-fabricated systems.

By performing high-resolution transmission electron microscopy imaging on lamellae made from 2D S/F stacks, we have established fabrication protocols under which good engagement between 2D S and 2D F flakes can be obtained – which is a key prerequisite to generate spin triplets' states at the 2D S/F interface.

The good engagement in our 2D S/F heterostructures is also demonstrated by measurements which we have carried out on tunneling devices [5] based on 2D S/F ($NbSe_2$/$CrGeTe_3$) vdW stacks, where we find clear evidence for a change in the density of states of $NbSe_2$ due to the proximity effect with $CrGeTe_3$.

From low temperature magnetotransport measurements on other types of 2D S/F devices, where we use a 2D F (i.e., $Cr_{1/3}NbS_2$) with an intrinsically inhomogeneous magnetization for spin triplet generation, we also find signatures for inverse superconducting proximity effects. These signatures include reentrant resistive states appearing in the resistance versus temperature curves of the 2D S/F bilayers (Fig. 1), which are also modulated by the applied field H, and a non-monotonic variation in the critical temperature Tc of the bilayers on the applied H, which is consistent with the generation of long-ranged spin-triplet pairs.

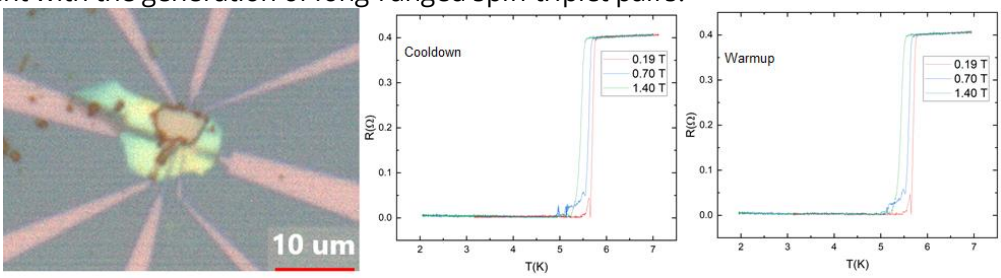

Figure 1: Optical microscope image of a $Cr_{1/3}NbS_2$/NbS_2 bilayer (left) and resistance versus temperature, $R(T)$, measurements showing a reentrant resistance behavior below the superconducting transition.

References:

[1] J. Linder, and J. W. A. Robinson, Nat. Phys. 11, 307-315 (2015).
[2] J.W.A. Robinson, J. D. S. Witt, and M. G. Blamire, "Controlled injection of spin-triplet supercurrent into a strong ferromagnet", Science 329, 59-61 (2010).
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Nr. 10: Interfacial helical currents in commensurate and tunable graphene-Bi_2Te_2Se heterostructures

Jonas Kiemle, Lukas Powalla, Katharina Polyudov, Maanwinder P. Singh, Alexander Holleitner, Marko Burghard, Christoph Kastl

Van der Waals heterostructures made from graphene and three-dimensional topological insulators promise very high electron mobilities, a non-trivial spin texture and a gate-tunability of the electronic properties. The above combination of advantageous electronic characteristics can only be achieved in such heterostructures, because graphene itself lacks a large enough spin-orbit interaction for measurable spin textures. In turn, the heterostructures are promising candidates for all electrical control of proximity-induced spin phenomena.

Here, we investigate epitaxially grown interfaces between graphene and the lattice-matched topological insulator Bi_2Te_2Se. Specifically, we study the spin-orbit coupling in the evolving van der Waals interfaces, which have been predicted to exhibit a highly anisotropic and electronically tunable spin texture. Polarization-resolved second harmonic generation, Raman-measurements, and time-resolved magneto-optic Kerr microscopies are used to demonstrate that the atomic interfaces align in a commensurate symmetry with characteristic interlayer vibrations. By polarization-resolved photocurrent measurements, we find a circular photogalvanic effect which is drastically enhanced at the Dirac point of the proximitized graphene. We attribute the helical currents to arise from the proximity-induced interfacial spin structure.

Nr. 11: Symmetries of ultrafast and interfacial currents in type-II Weyl semimetal candidates and their heterostructures

Maanwinder Partap Singh, Jonas Kiemle, Lukas Powalla, Elio König, Andreas Schnyder, Alexander Holleitner, Marko Burghard, and Christoph Kastl

The layered van der Waals materials $MoTe_2$ and WTe_2 are potential candidates to realize topological type-II Weyl semimetals. Topological phases with strong spin-orbit couplings and low crystal symmetries, in particular $MoTe_2$ and WTe_2, can enable an efficient optical and electrical manipulation of spin currents in van der Waals heterostructures.

For $MoTe_2$, we address the impact of crystal phase disorder on the generation of helicity-dependent photocurrents. Using scanning photocurrent microscopy, we spatially probe the phase transition and its hysteresis between the centrosymmetric, monoclinic 1T' phase to the symmetry-broken, orthorhombic Td phase as a function of temperature. We demonstrate that ultrafast, helicity-dependent photocurrents in $MoTe_2$ arise most likely from a local breaking of the electronic symmetries due to phase disorder.

In graphene/WTe_2 heterostructures, we study the possibility to induce current-driven and gate-tunable spin polarisations. For the detection of the spin polarisation, we employ magneto-optical Kerr microscopy. Even for a nominal in-plane transport, substantial out-of-plane spin accumulation is induced by a corresponding out-of-plane current flow. We present a theoretical model which fully explains the gate- and bias-dependent onset and spatial distribution of the intense Kerr signal as a result of a non-linear anomalous Hall effect in the heterostructure, which is enabled by its reduced point group symmetry.

Our results highlight the impact of local crystal symmetries on the generation of ultrafast charge and spin current in van der Waals heterostructures [1,2].

References:

[1] M. P. Singh et al. 2D Mater. 9 011002 (2022).
[2] L. Powalla et al. arXiv preprint arXiv:2106.15509 (2021).

Nr. 12: The Importance of Relaxation Effects on the Properties of Twisted van der Waals Materials

Florian M. Arnold, Alireza Ghasemifard, Agnieszka Kuc, Jens Kunstmann, Thomas Heine

The stacking of single layer 2D crystals, such as transition-metal dichalcogenides, creates a new class of materials: van der Waals [hetero]structures. [1] In these materials, a variety of structures can be realized by controlling the stacking order and the twist angle between adjacent layers. In our work, the influence of the twist angle on the structural and electronical properties of MoS_2 bilayers was studied using reactive force field (ReaxFF) and density functional theory (DFT) calculations.

Interlayer twisting leads to the formation of moiré patterns of rapidly increasing size with decreasing twist angles towards 0° and 60°, resulting in huge simulation cells that are only accessible computationally using force fields. [2] This concept of constructing twisted bilayers, by a rigid rotation between the individual layers, is used in many studies. However, it neglects the importance of relaxation effects – these result in a significant deformation of the individual layers, especially for small twist angles, and strong changes of the interlayer distance in different areas of the structure. Our work gives a detailed overview of the influence of relaxation on the structural properties in such systems and how different structural regimes – soliton, transition, and moiré regime – form depending on the interlayer twist angle. We further demonstrate how these changes can strongly influence the analysis of electronic properties, as shown in the Figure 1, thus emphasizing the need for thorough relaxation in computational studies of van der Waals [hetero]structures. [3]

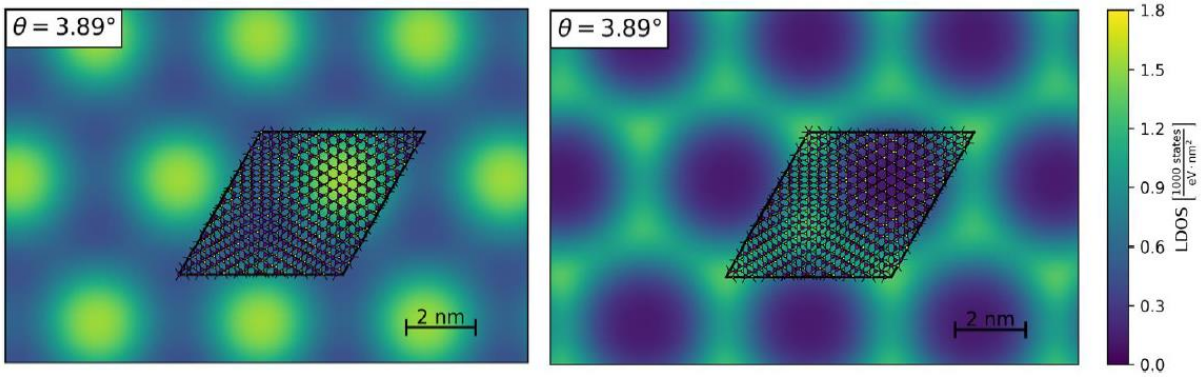

Figure 1: Atom-projected density of states map in the valence band region (E = -0.268 eV) of a bilayer MoS_2 with a twist angle of 3.89°. The atomic structure is included for the primitive moiré cell. In the case of (left) rigidly twisted layers the valence band is localized in strongly confined regions. Extensive changes can be observed in the case of (right) a fully relaxed structure where a delocalized hexagonal network, associated with the appearance of strain solitons, is formed.

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Nr. 13: Single skyrmion generation in vdW heterostructures based on the 2D magnet Fe_3GeTe_2

Sayooj Satheesh, Lukas Powalla, Max Birch, Kai Litzius, Gisela Schütz, Marko Burghard

Topological spin textures like skyrmions hold great promise for the further development of the field of spintronics. Owing to their atomically flat surfaces and their capability to be smoothly integrated in vdW heterostructures, the recently discovered 2D van der Waals (vdW) magnets are especially promising for achieving efficient skyrmion generation, manipulation and detection. As a first step toward the controlled, local formation of skyrmions in the 2D magnet Fe_3GeTe_2 (FGT), we have utilized real-space imaging to determine thickness-dependent magnetic phase diagrams of exfoliated FGT sheets. It turned out that the unique material properties of FGT result in a complex, history-dependent emergence of the uniformly magnetized, stripe domain and skyrmion states. This enables the stabilization of all these states at zero field, and at a single temperature. In addition, based upon the comparison to magnetic simulations, we elucidate the interplay of interactions governing the skyrmion formation. Furthermore, we demonstrate that heterostructures combining FGT with a graphite top electrode are highly suitable for single skyrmion generation. Specifically, upon step-wise increasing the voltage applied between FGT and graphite layers, a vertically conducting pathway is formed, which enables skyrmion nucleation through a local heating-based mechanism.

Nr. 14: Strain control of moiré lattice geometry on homo and hetero bilayers of transition metal dichalcogenides.

Pedro Soubelet, Maximilian Kögl, Mauro Brotons-Gisbert, Andreas V. Stier, Brian Gerardot, and Jonathan J. Finley

Twisted van der Waals (vdW) homo- and heterostructures have received prominent attention for their capability of supporting strongly correlated quantum phases [1]. However, the appearance of topological features and emergent many body quantum phases is highly sensitive to the strength, periodicity and symmetry of the underlying moiré potentials, delicately defined by the relative misalignment of the constitutive layers. The strong dependence on stacking angle and the difficulty to modify the structure once fabricated make the reproducibility of results extremely arduous and, therefore, the development of a dynamic tuning technique is mandatory to achieve a full understanding of the spectrum of accessible physics. In this context, strain has been proposed as a tuning knob to give the system an extra degree of freedom to control, in situ, electronic properties of the vdW structures [2,3]. In this contribution, we study the effect of heterostrain on moiré lattice in homo- and heterobilayers of transition metal dichalcogenides systems. In particular, we show that the application of a small uniaxial and biaxial heterostrain (±2%) leads to strong variations in the moiré lattice periodicity and geometry, facilitating the creation, for instance, of rectangular moiré lattices. Our results show the advantage of heterostrain control towards possible technological applications that utilize, on demand, quantum phases in a quantum simulator platform.

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Nr. 15: Probing the local dielectric function of WS_2 on an Au substrate by near field optical microscopy operating in the visible spectral range

O. Garrity, A. Rodriguez, N. S. Mueller, O. Frank, and P. Kusch

The optoelectronic properties of 2D systems such as transition metal dichalcogenides (TMDs) are characterised by the complex, frequency dependent dielectric function. The dielectric function is influenced by several factors such as excitonic resonances, charge transfer effects, and sample contamination. The presence of interlayer excitons in a heterobilayer made up of two different TMDs should also affect the local dielectric function of the sample. This work aims to use scanning type near field optical microscopy (s-SNOM) to characterise local dielectric variations of a sample at the nanometre length scale and extract the overall dielectric function from different depths of the sample/substrate. We studied a monolayer of WS_2 on Au substrate and used the s-SNOM to identify two areas of differing levels of charge transfer. Then, using a pre-established inversion method we extracted dielectric values from different penetration depths of the sample and compared them to dielectric values obtained via spectroscopic imaging ellipsometry (SIE). These experiments highlight the advantage of this technique in that samples with dirty or contaminated areas can be identified and eliminated [1]. It can also be used to study the effect of localised interlayer excitonic states on the dielectric function of TMD heterobilayers.

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Nr. 16: Spatial Control of Graphene Functionalization by Patterning a 2D Substrate

Tobias Dierke, Janina Maultzsch

We present an experimental study on the degree of covalent functionalization of exfoliated graphene on top of alternating hBN and Si/SiO_2 stripes. The underlying substrate has a strong effect on the degree of functionalization of graphene. Our results show that the functionalization of graphene is less effective on hBN compared to SiO_2, resulting in higher defect-induced modes in the Raman spectra on SiO_2.
Other underlying 2D materials like MoS_2, WS_2, and MoO_3 show less contrast in functionalization density than hBN or lead to even higher degree of functionalization than the underlying Si/SiO_2 substrate.
Patterning the underlying substrate is therefore a versatile method for spatially defined functionalization of graphene, as it preserves the intrinsic high-quality properties of graphene compared to other patterning approaches.

Nr. 17: Optical properties of 2D tungsten-disulfide/-diselenide heterobilayers

Manan Shah, Mohammed Adel Aly, Eui-Hyeok Yang, and Arash Rahimi-Iman

The opportunity of vertically stacking 2D materials without lattice-matching constraints has further enriched semiconductor spectroscopy with the possibility to investigate twist- or stacking-configuration related optoelectronic heterostructure (HS) properties. Most prominent are investigations on excitonic features in monolayers (ML) and their heterobilayers (HBLs), particularly with the aim of studying charge-transfer excitons that may arise as spatially-separated interlayer species with Coulomb interactions across the interface. Furthermore, band-hybrid bilayer features are understood to occur, as well as peculiarities induced by periodic potential landscapes (moiré patterns), i.e. emission behavior attributed to the nanoscale naturally-formed superlattices for arbitrary twist angles.

In fact, the interlayer exciton which can be formed in HBLs as a result of type-II band alignment configurations received much attention in recent years, owing to the straight-forward achievement of ML-ML stacking, promising long-living excitons with dipolar character and layer-separation of charge carriers for photonic applications. Here, a study of emission properties, which extends our ongoing optical characterization of the abundant excitons in these well-accessible and excitons-rich tungsten-based HBLs, is summarized. Future time- and angle-resolved characterization of high-quality 2D interfaces may provide further insights into the properties of excitons reentering the 3D world from their 2D-materials system.

Nr. 18: Corrugation in twisted transition metal dichalcogenide heterostructures

Wei Li, Thomas Brumme

The interlayer van der Waals (vdW) interactions enable two single layers of a two-dimensional material to vertically stack together and form van der Waals heterostructures (vdWHs). If the two layers have different distinct symmetries or lattice sizes or if they are twisted with respect to each other, a moiré pattern with much larger length scale than the periodicity of each layer is formed. In order to fully understand the optical and electronic properties of these heterostructures the structural changes on the scale of the moire supercell need to be included. Here we performed structure relaxation for $MoS_2/MoSe_2$ vdWHs using the force-field method employing the Stillinger-Weber (SW)[1] and Kolmogorov-Crespi (KC)[2] potential to capture the intralayer and interlayer interaction. Significant out-of-plane deformation can be observed and both layers corrugated remarkably, which can be modified by twist angle. Domain patterns are formed, where areas with matching lattice constants are separated by node and domain walls that accumulate the generated strain.

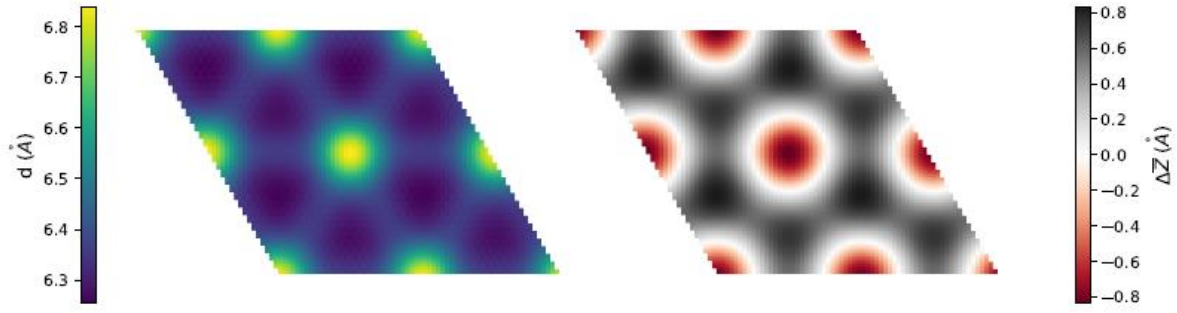

FIG. 1. Interlayer distance d of $MoS_2/MoSe_2$ vdWHs, defined as the distance between the two adjacent surfaces generated by the metal atoms. Average out-of-plane displacement $\Delta\bar{Z}$, defined as the average of the out-of-plane displacement of metal atoms in two adjacent layer by interpolation.

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Nr. 19: Edge states in proximitized graphene ribbons and flakes in a perpendicular magnetic field: emergence of lone pseudohelical pairs and pure spin-current states

Yaroslav Zhumagulov, Tobias Frank and Jaroslav Fabian

Graphene influenced by the valley-Zeeman intrinsic spin-orbit coupling through proximity effects provides signatures of pseudohelical edge states [1,2]. Analyzing the band structure of a zigzag graphene nanoribbon in the presence of proximity induced spin-orbit interaction and an external magnetic field, we have discovered the effect of stabilization of intervalley edge states and removal intravalley edge states by the external magnetic field. Stabilization of states is associated with the closing/reopening of the bulk bandgap between nonzero Landau levels [3]. The magnitude of the external magnetic stabilization field was estimated both numerically and analytically. Finally, we have found that stabilized intervalley edge states in the presence or in the absence of a spin-flip hopping through the armchair edge form pseudohelical states or pure spin current states, respectively. The states of pure spin current are formed in wide graphene flakes and are protected from scattering by defects on the zigzag edges of graphene flakes.

This work was supported by DFG SPP 2244, DFG SFB 1277 and EU Graphene Flagship.

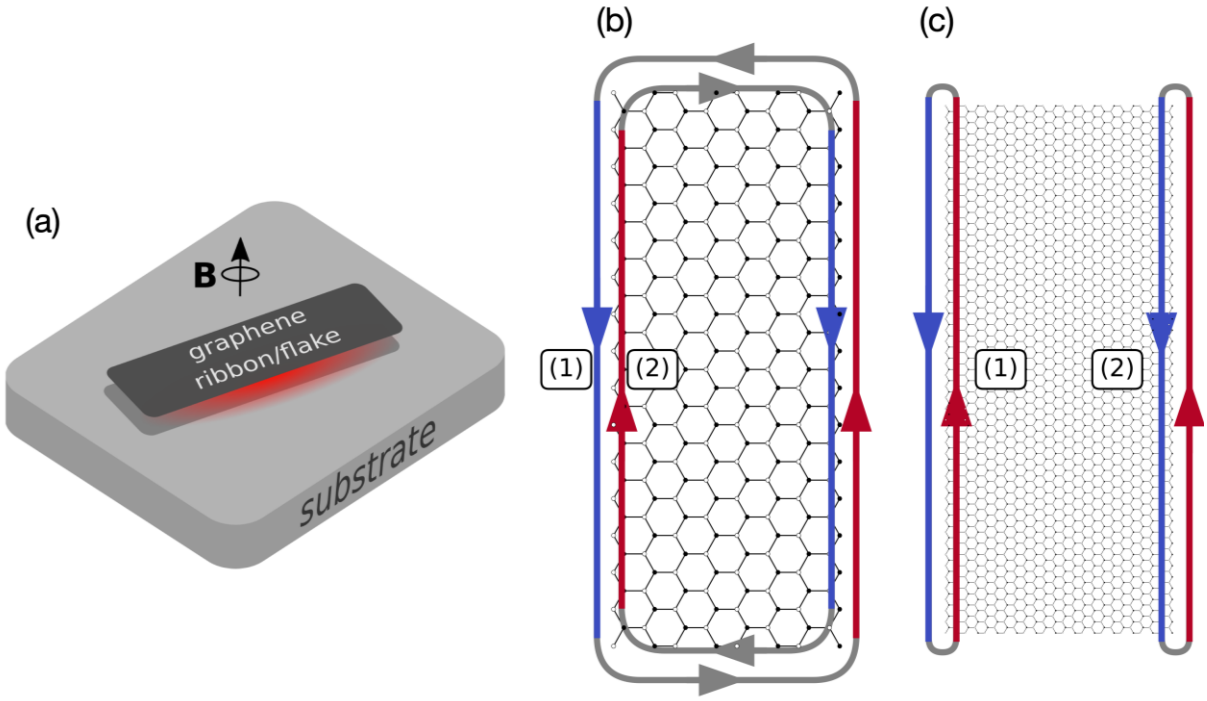

Figure 1: (a) Side view of graphene/TMDC heterostucture with proximity effect in a magnetic field. Schematic representation of pseudohelical states (a) and pure spin current states (b).

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Nr. 20: Quantum gases in semiconductor van der Waals heterostructures

Jonas Göser, Edith Wietek, Ruven Hübner, Alexander Högele, Alexey Chernikov, Alexander Steinhoff

In our project we aim to explore the paradigms of composite quasiparticle quantum gases in the framework of van der Waals heterostructures. Our combined experimental and theoretical efforts focus on many-body interactions beyond the composite boson picture of individual interlayer excitons towards dense Fermi-Bose mixtures and increasingly exotic regimes of correlated electron-hole plasma representing mixed Fermi liquids. We report progress along these lines of research, achieved in both experiment and theory. Experimental aspects include studies of vertical heterobilayers such as $MoSe_2/WSe_2$ fabricated by mechanical exfoliation stacking or via chemical vapor deposition synthesis. Due to lattice mismatch or in the presence of finite twist, they represent canonical moiré heterosystems as hosts for dipolar exciton gases. For marginally twisted systems, our experimental studies with optical spectroscopy suggest a lattice transformation from ideal moiré periodicity to mesoscopically reconstructed domains. In the presence of large-scale reconstructed domains, we find evidence of interlayer excitons in linear reflectance and determine a comparatively large oscillator strength of about 2% compared to the intralayer states. Moreover, using transient microscopy we observe efficient propagation of interlayer excitons indicating phonon-limited diffusion and find absence of localization even at lowest studied temperature of 5 K and strong evidence for free exciton transport. In theory, we started to develop adequate models for electronic and optical properties of TMD heterostructures following two complementary pathways. First, in collaboration with external partners, we extended the established Wannier-based description of single-particle states and screened Coulomb interaction to bilayers with fixed stacking order. The resulting ab initio-based description is used to establish a many-body theory of optical response and, prospectively, of exciton ionization. Secondly, a tight-binding description for low-energy bands in twisted TMD heterobilayers was developed. We used a Slater-Koster based inter-layer coupling Hamiltonian to describe hybridization effects and obtain access to twist-dependent energy renormalizations.

Nr. 21: Two-color time-resolved Kerr rotation measurements of TMDC heterostructures

Michael Kempf, Maximilian Tomoscheit, Annika Bergmann, Johannes Reinhold, Mustafa Hemaid, lina Schubert, Antony George, Andrey Turchanin, Rico Schwartz, and Tobias Korn

Transition metal dichalcogenides (TMDC) have revealed many intriguing properties in recent years. For valleytronics especially, the coupling of spin and valley degrees of freedom shows great promise. Using valley-selective optical selection rules, a coupled spin-valley polarization can easily be introduced in these systems. Keeping possible future applications in mind, the dynamics of this polarization, especially its lifetime, is of great importance. Yet in pristine monolayer TMDCs the lifetime is strongly limited due to ultrafast optical exciton recombination and electron-hole exchange interaction. By contrast, in TMDC heterostructures, ultrafast interlayer charge transfer may circumvent these limits on valley polarization lifetimes. We use two-color time-resolved Kerr rotation measurements to study the spin-valley dynamics in disulfide-based TMDCs and their heterostructures. The independent tunability of our coupled laser systems allows to selectively pump and probe their excitonic transitions resonantly. We present low-temperature valley dynamics studies on TMDC monolayers and twisted MoS_2-WS_2 heterostructures fabricated by combining CVD-grown and exfoliated monolayers.

Nr. 22: Interlayer excitons in advanced, CVD-based van der Waals heterostructures with controlled moiré potentials: $MoSe_2$-WSe_2 structures

Andreas Beer, Anna Weindl, Laura Zinkl, Kenji Watanabe, Takashi Taniguchi, Antony George, Andrey Turchanin, and Christian Schüller

In our common project, together with the groups of Tobias Korn in Rostock and Andrey Turchanin in Jena, our focus is the investigation of the temporal and spatial dynamics of interlayer excitons in MoSe2-WSe2 heterostructures with well-defined moiré potentials, based on CVD grown samples. The so called hot pickup method enables us to fabricate such heterostructures out of CVD grown triangulars in a controlled, dry, PDMS-free and easy way. We observe homogeneous interlayer exciton photoluminescence and a drastic intralayer photoluminescence quenching in the heterostructure region.

The high quality of the heterostructures is also characterized by the observation of characteristic Raman modes, like moiré phonon modes or interlayer shear modes. First measurements on exfoliated heterostructures reveal twist-angle-dependent decay times of the interlayer exciton.

Furthermore, we compare exfoliated and CVD-grown $MoSe_2$ and WSe_2 monolayers, encapsulated in hexagonal Boron nitride. The results show the high quality of the CVD-grown monolayers.

Nr. 23: Preparation of high-quality TMDs by chemical vapor deposition for optical applications

Julian Picker, Ziyang Gan, Antony George, Andrey Turchanin

Monolayer transition metal dichalcogenides (TMD) (e.g.: MoS_2, WSe_2, $MoSe_2$, WSe_2, $NbSe_2$, etc.) have attracted significant research interest in recent years owing to their unique electronic and optical properties for potential applications in ultrathin device technology. TMD monolayers are available as n-type semiconducting ($MoSe_2$, MoS_2, WS_2), p-type semiconducting (WSe_2), metallic ($NbSe_2$, NbS_2), and as semi metallic (WTe_2) materials. To enable the applicability of these ultrathin monolayers, it is essential to develop efficient large area synthesis techniques. In this poster, we present tailored synthesis of high-quality monolayer TMDs by chemical vapor deposition. The grown TMDs were characterized in detail using complementary characterization tools including optical microscopy, atomic force and scanning tunneling microscopy, Raman spectroscopy, and X-ray photoelectron spectroscopy to understand their structural and chemical properties. By performing low temperature optical spectroscopy, the high optical quality of the CVD grown monolayers is revealed. The nature of defects and defect density were investigated using high resolution transmission electron microscopy. The influence of defects in the electronic and optoelectronic properties were investigated using electrical transport measurements and scanning tunneling spectroscopy. Furthermore, we succeeded in depositing TMDs on a single crystal Au(111) surface. By means of surface sensitive ultra-high vacuum methods we measured the electronic and structural properties of such single crystalline TMDs down to atomic scale.

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Nr. 24: Subnanoscale Engineering of 2D Magnetism in van der Waals Heterostructures

Keda Jin, Jose Martinez-Castro, Stefan F. Tautz, Markus Ternes

Dry transferred method paves a way to investigate exotic properties and emerging new phenomena in van der Waals heterostructures.[1] Polycarbonate (PC) [2] is commonly used as a polymer for the dry transfer of 2D materials. A limitation of PC is the contamination of chemical residues on the surface [3] and the difficulty to fabricate complex heterostructures [4]. Here, we show the study of different polymers, including polyvinyl chloride (PVC) [5] and nitrocellulose [4,6] for an effective and clean way to assemble 2D heterostructures. In addition, based on our previous method of studying encapsulated air sensitive 2D materials[7], we show our current development in a new technique to study air-sensitive materials in heterostructures compatible with ultra-high vacuum: in-situ de-encapsulation. This technique aims to provide the required cleanliness of mechanical assembled air sensitive van der Waals heterostructures for their study by scanning tunneling microscopy at ultra-high vacuum and low temperature in the next step of our project.

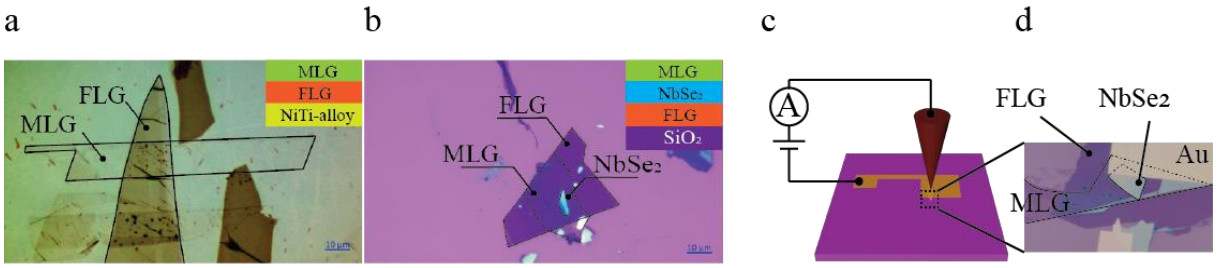

Fig 1. (a) Nitrocellulose transferred vdW heterostructure on a NiTi alloy, and (b) on a SiO2 substrate. (c) Scheme of our set-up for in-situ deencapsulation, and (d) the corresponding optical image of the sample.

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Nr. 25: Magnetism in two-dimensional $CrTe_2$

Nihad AbuAwwad, Manuel dos Santos Dias, Samir Lounis

The discovery of two-dimensional (2D) van der Waals magnets opened unprecedented opportunities for the fundamental exploration of magnetism in quantum materials and the realization of next generation spintronic devices. Recently, thin $CrTe_2$ films were demonstrated to be ferromagnetic up to room temperature, with an intriguing dependence of the easy axis on the thickness of the material [1,2]. On the other hand, a zig-zag antiferromagnetic state has been observed by spin-polarized scanning tunneling microscopy in a monolayer [3]. Here, we demonstrate using first principles a strong coupling between magnetism and structure in a single layer of $CrTe_2$ through calculating the magnetic interactions. Also, utilizing atomistic spin dynamics, we perform a detailed investigation of the complex magnetic properties pertaining to this 2D material.

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Nr. 26: 2D quantum materials on demand: twisting, stacking & gating

Nihit Saigal, Hossein Ostovar, David Tiede, Torsten Stiehm, Hendrik Lambers, Ursula Wurstbauer

Two-dimensional (2D) quantum materials are of increasing interest because they host controllable quantum states and emerging phases. Emergent phases such as magnetism, superconductivity, superfluidity or Mott insulator states are driven by interactions. Interactions in those systems can be engineered by stacking different 2D layered materials together by precisely adjusting the twist angles in between, by application of electric or magnetic fields or by degenerately doping them e.g. via field effect doping. In order to study the fascinating physics of emerging quantum phases in twisted or electric-field gated TDMC by millikelvin interband magneto-optics and resonant inelastic light scattering on low-energy collective excitations, we optimized field effect structures for high electron and hole doping densities up to 1014 cm^{-2} suitable for optical measurements and enabling all optical electrolyte gate spectroscopy to determine the single particle band gap [1]. Moreover, ultra-low frequency resonant and non-resonant Raman experiments on twisted hetero-bilayer at millikelvin temperatures have been established. We demonstrate by means of Raman measurements that a connected heterobilayer can have commensurate stacked and twisted regions and can correlated the twisted region with emission from Moiré excitons [2]. Shape and energy of Resonant Raman modes only apparent at ultra-low temperatures suggest coupling between vibrational and collective charge degrees of freedom.

We acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under projects Wu 637/ 7-1 and SPP 2244.

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Nr. 27: 1D topological superconductivity and Majorana states in van der Waals heterostructures characterized by scanning probe microscopy

Tobias Wichmann, Felix Lüpke

Topological superconductivity is an exotic state of matter with potential applications in quantum computing. A promising approach to realize topological superconductivity is to use a conventional superconductor to induce superconductivity in a topological edge state via the superconducting proximity effect. Using a newly developed sample fabrication technique, the ‘dry-transfer flip technique’, as well as epitaxial thin films which are grown by our collaborators, we propose to create van der Waals (vdW) heterostructures of two-dimensional, atomically thin layers of topological insulators on superconductors. Using scanning probe microscopy at low temperatures and in ultra-high vacuum, we then characterize the induced superconductivity in the topological edge state. By combination of a topological superconductor with some form of magnetism, e.g. a magnetic layer, a magnetic cluster or by application of an external magnetic field, so-called Majorana quasi-particles can be created in the topological superconductor. We propose to realize and study Majorana states created in the vdW heterostructures to gain a deeper understanding of the underlying physics. Another sample system in which we propose to realize Majorana states are atomically thin layers of $NbSe_2$ which are placed on a vdW magnet such as Fe_3GeTe_2.

Nr. 28: Optical excitations in transition metal dichalcogenides under pressure

Paul Steeger, Jan-Hauke Graalmann, Robert Schmidt, Philipp Marauhn, Marie-Christin Heißenbüttel, Jan Nellesen, Ilya Kupenko, Carmen Sanchez-Valle, Steffen Michaelis de Vasconcellos, Michael Rohlfing, Rudolf Bratschitsch

Multilayer stacks of 2D semiconductors in the form of hetero- and homo-structures possess great potential to extend Moore's law by replacing traditional semiconductors in (opto-)electronic devices and to develop completely new devices based on effects such as valley physics or moiré excitons. One of the most critical parameters in homo- and heterostructures is the interlayer coupling between electron and holes across the different layers, strongly affecting the electronic and optical properties of the system.

One key parameter that influences the interlayer coupling strength is the distance between adjacent layers, which can be controlled by applying pressure to the layered crystal. Here, we investigate experimentally and theoretically the optical properties of bilayer and bulk (few-layer) MoS2 under (hydrostatic) pressure. The prototypical 2D semiconductor MoS_2 is well suited as a model system, as it features an interlayer exciton with a considerable oscillator strength at room temperature, being an indicator of the interaction between the individual layers in a multilayered crystal.

We prepare bilayer and few-layer MoS2 by micromechanical exfoliation from bulk crystals and measure stationary optical absorption and transient transmission spectra of intralayer (A and B) and interlayer excitons depending on pressure in a diamond anvil cell. We find a distinct change of the intralayer and interlayer exciton energies and a strongly modified ultrafast dynamics.

Structural deformations by hydrostatic stress are explored using ab initio van der Waals-corrected DFT-PBE calculations, revealing the competition between in-plane and out-of-plane compression on the atomic positions, leading to a non-linear behavior already at relatively low pressure. The band structure and optical excitations of the deformed MoS_2 are calculated with the GW method and its highly efficient LDA+GdW version, and by solving the Bethe-Salpeter equation. Our theoretical investigations show a non-linear gauge factor, which is different for the A and interlayer exciton. This is explained by the different extension of the wave function in real space, as well as by the sensitive dependence of the excitons on details of the geometric structure.

Nr. 29: Structure and nanomechanics of MoS_2/graphene/SiC van der Waals heterostructures

Bartosz Szczefanowicz, Zhao Liu, Marcelo Lopes, Antony George, Roland Bennewitz

Friction on 2D materials can be tuned by number of layers [1], application of electric bias[2] and combination of different materials into one van der Waals heterostructure [3]. We hypothesize that a compensation of the contact potential can minimize friction on heterostructures of MoS_2 on epitaxial graphene on SiC(0001). 2D MoS_2 was grown via CVD on epitaxial graphene which was previously grown from SiC(0001). Material contrast and the number of layers was revealed by Atomic Force Microscopy (AFM) and Kelvin Probe Force Microscopy (KPFM). Load and bias dependencies of friction force on different variants of heterostructures were measured by means of Friction Force Microscopy (FFM). Single MoS_2 triangles could be moved to positions of interest by means of the scanning tip. The MoS_2 graphene system is also investigated with respect to the formation of intermittent covalent bonds induced by the high pressure under the AFM tip.

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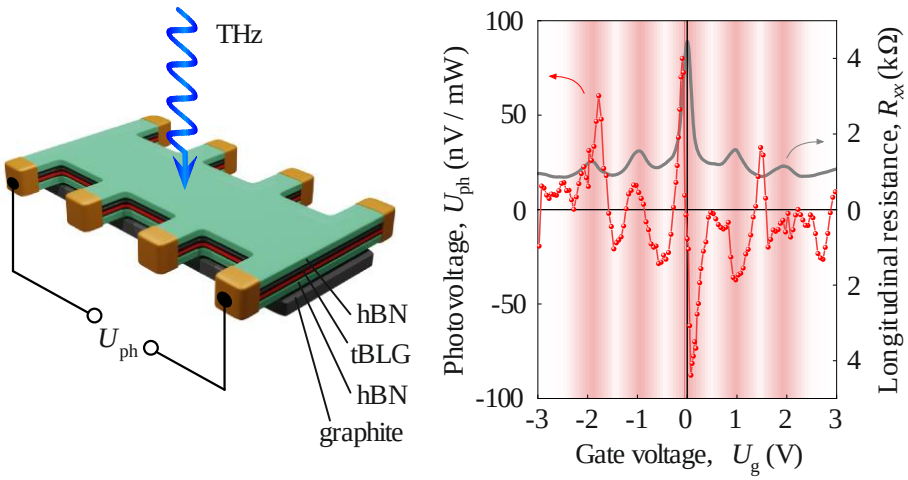
Nr. 30: Nonlinear photocurrents induced by terahertz radiation in twisted bilayer graphene

S. Hubmann, P. Soul, G. di Battista, M. Hild, L.E. Golub, K. Watanabe, T. Taniguchi, X. Lu, D.A. Kozlov, D.K. Efetov, and S.D. Ganichev

We report on the observation of nonlinear photocurrent and photoconductivity in twisted bilayer graphene (tBLG) with twist angles below 1°. We show that excitation of the tBLG bulk causes a photocurrent, whose sign and magnitude are controlled by the orientation of the radiation electric field and the photon helicity. The observed photocurrent provides evidence for the reduction of the point group symmetry in low twist-angle tBLG to the lowest possible one. The developed theory shows that the current is formed by asymmetric scattering in gyrotropic tBLG. We also detected the photogalvanic current formed in the vicinity of the edges. For both bulk and edge photocurrents, we demonstrate the emergence of pronounced oscillations upon variation of the gate voltage, which correlate with the oscillations of the sample resistance. These photocurrent oscillations are explained by interband transitions between a multitude of isolated bands in tBLG.

Furthermore, at higher radiation intensities, we detected a nonlinear intensity dependence of the bulk photogalvanic current and the photoconductivity. These nonlinear photoresponses are caused by the interplay between direct interband transitions, optical transitions between Moiré subbands, and indirect optical transitions (free carrier absorption). This interplay is controlled by the Fermi level position with respect to the Moiré subbands. We show that the photosignals saturate with rising intensity, while contributions from different transitions differ in their respective saturation behavior.



Left: Sketch of the experimental setup. Right: Photocurrent (red) and resistance (gray) oscillations with the gate voltage.

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Nr. 31: Moiré Engineering of Spin-Orbit Coupling in Twisted Platinum Diselenide

Lennart Klebl, Qiaoling Xu, Ammon Fischer, Lede Xian, Martin Claassen, Angel Rubio, Dante M. Kennes

We study the electronic structure and correlated phases of twisted bilayers of platinum diselenide using large-scale ab initio simulations combined with the functional renormalization group. PtSe2 is a group-X transition metal dichalcogenide, which hosts emergent flat bands at small twist angles in the twisted bilayer. Remarkably, we find that moiré engineering can be used to tune the strength of Rashba spin-orbit interactions, altering the electronic behavior in a novel manner. We reveal that an effective triangular lattice with a twist-controlled ratio between kinetic and spin-orbit coupling scales can be realized. Even dominant spin-orbit coupling can be accessed in this way and we discuss consequences for the interaction driven phase diagram, which features pronounced exotic superconducting and entangled spin-charge density waves.

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Nr. 32: Chasing Polaritons: A Pathway to investigate the optoelectronic properties of van der Waals heterostructures

Oisin Garrity, Patryk Kusch and Stephanie Reich

Transition metal dichalcogenides (TMDs) possess a rich amount of exciting fundamental physics to explore, chief among them is their excitonic physics. With strong binding energies (50-200 meV) at room temperature, band gaps in the visible to the infrared, and both direct and indirect bandgap configurations possible [1], they are excellent materials for the study of excitons and how they interact with light. Our project aims to explore the fundamental physics of interlayer excitons and exciton polaritons, formed when two 2D layers are stacked upon each other (heterostructure). We envision gaining access to their lifetime transition energy and light matter coupling.

To understand light matter interaction in heterostructures, we began by investigating exciton polaritons in thin molybdenum disulphide (MoS_2) slabs by imaging their optical near field using scanning type near field optical microscopy (s-SNOM) and a fully tuneable laser in the visible for excitation [1]. By measuring the dispersion relation of polaritons formed by the A and B we demonstrate that the exciton polaritons strongly couple with with a coupling strength of 40 meV for the A and 100 meV for the B exciton.

We introduce the s-SNOM as a fast and reliable tool for the identification and imaging of areas in 2D heterostructures, where interlayer excitons are formed, that was challenging so far. To that end, we study the influences excitonic resonances have on the local dielectric properties of the TMDs, we used s-SNOM to identify areas of differing dielectric environments and by utilising a pre-established inversion method to extract the local dielectric function of the sample on the nanometre scale [2]. Second, we demonstrated an anticorrelation between near field amplitude recorded in with the s-SNOM and tip-enhanced photoluminescent (TEPL) [2]. Finally, we succeeded to image by s-SNOM areas on 2D heterostructures that exhibits interlayer excitons. We backup our observation with PL and kelvin probe force microscopy.

One main challenge for our project is still to get a large number of high-quality samples. To tackle this, we started a collaboration with Professor Tobias Korn of the University of Rostock. In Rostock we were introduced to the transfer setup they made to produce heterostructures and made two $MoSe_2$/WSe_2 heterostructures to take with us. These samples were used for s-SNOM imaging and resonant Raman experiments that allow to study electronic and vibronic properties of heterostructures. We observe a red shift in excitonic resonance in the heterostructure when compared to their monolayer counterparts. Similar results were recently published that indicate this is a result of stronger dielectric screening in the heterostructure in comparison to the monolayers [4]. Furthermore, we observe a second resonance that appears between the $MoSe_2$ and WSe_2 resonances, which requires further investigation. The results will be summarized in a publication. Finally, taking inspiration from the example shown to us in Rostock, we build up our own transfer setup and are beginning to make our own heterostructures.

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Nr. 33: Neutral excitons and exchange-split trions dynamics engineered by strain in monolayer WSe_2

Zhao An, Pedro Soubelet, Michael Zopf, Andreas V. Stier, F. Ding, and Jonathan J. Finley

Semiconducting transition metal dichalcogenides (TMDs) are layered materials with promising applications in optoelectronics and spintronics, turning them into ideal building blocks to control spin and valley degrees of freedom. In the monolayer limit, they exhibit remarkably strong light-matter interaction driven by tightly bound excitons. In optically dark monolayer TMDs, like WSe_2 and WS_2, the optical excitation with circularly polarized light gives rise to excitonic complexes that exhibit photoluminescence with cross-polarized emission [1,2]. This effect arises from an intricate interplay between the efficient spin/valley pumping of resident electrons and the intervalley scattering of electrons and neutral excitons [2]. In this contribution, we use a piezoelectric device to apply, on-demand, biaxial strain to WSe_2 monolayers and explore inter- and intravalley trions. In particular, polarization resolved photoluminescence experiments reveal non-trivial strain effects on the singlet-triplet trion splitting and also on the degree of circular polarization of all bright and dark excitonic complexes observed.

Strain engineering is a powerful tool to modulate the electronic bands of a two-dimensional material and tune a variety of physical properties. Our results shed light on the excitonic interlayer scattering and the electron-electron exchange interaction strength that define the energy and formation dynamics of singlet and triplet trion configurations in the material.

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Nr. 34: Transport Measurements in Twisted Graphene Heterostructures around the Magic Angle

B. Zheng, X. Zhang, J. Huang, L. Thole, L. Bockhorn, and R. J. Haug

The stacking and folding angle of 2D materials to 3D structures has emerged as an important, novel tuning parameter for the tailoring of optical, mechanical, electronic and magnetic properties. Especially, the electronic properties of twisted (double) bilayer graphene strongly depend on relative orientation of the two atomic lattices [1, 2]. These heterostructures were the first systems to show new many body phases in graphene, as e.g. superconductivity or Mott insulator phases [3].

We fabricate twisted bilayer/multilayer graphene sample which are encapsulated by hexagonal boron nitride via dry release transfer method und investigate the electronic properties under low temperature and high magnetic field, especially the quantum Hall effect.

The new many body phases were observed at the first magic angle 1.1° in twisted bilayers of graphene (see Fig. 1). In addition, there should exist similar magic angles with flat bands [4] at angles of 0.5°, 0.35°, 0.24° and 0.2°. Such small angles are extremely difficult to produce with the current transfer techniques for graphene heterostructures. Strain which works in a similar way as tuning the twist angle (see Fig.2) would offer the chance to investigate many body phases for these new flat band conditions. Anisotropic strain produced via piezo will give an additional twist to this phase diagram.

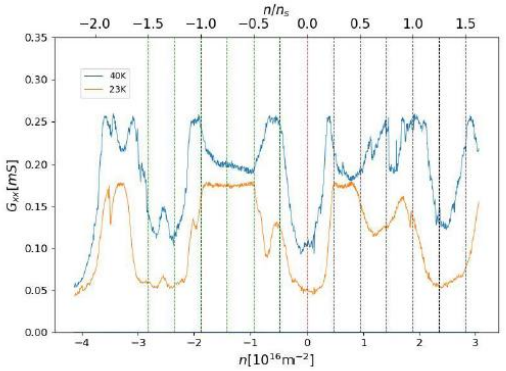

Fig.1: The longitudinal conductance of a 0.9°-TBG sample changes periodically with the charge carrier density at low temperature.

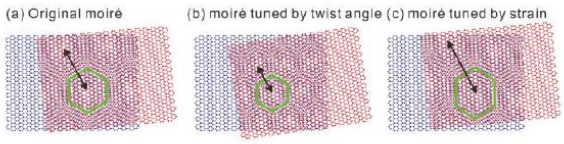

Fig.2: (a) Original moiré pattern (b) moiré pattern tuned by twist angle (c) moiré tuned by applying strain

In electrical transport measurement, the superlattice in a TBG can be identified by the appearance of satellite peaks in Land au fan diagram, superconductivity by vanishing resistance, Mott transitions by diverging resistances.

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Nr. 35: Topological effects in graphene/2D polymer superlattices

Francesca Falorsi, Kejun Liu, Miroslav Polozij, Thomas Heine, Xinliang Feng, Thomas Weitz, Renhao Dong

Stacking two or more 2D crystals of the same or of different kinds to so-called van-der-Waals hetero-structures triggers strong interlayer effects, allowing access to new and interesting physical phenomena. Recently, a new class of 2D materials has emerged, namely crystalline 2D polymers (C2DPs). In C2DPs, molecular building blocks are stitched together by strong covalent bonds, and they are formed in different lattice topologies, which directly impacts the electronic band structure. This work aims to explore the proximity effect caused physics of HSs formed by graphene and C2DPs. These novel materials coupled to graphene, or other 2D crystals are expected to generate a large range of new physical phenomena, including structural and electronic moiré patterns, impact on the graphene band structure (including band gap opening and band flattening), magnetic superlattices, and possibly many more. Initially, HSs formed by a C2DP that comprises metal-free porphyrin and perylene units linked by imide bonds, and graphene, transferred on the COF with dry transfer method, is studied. The Raman spectra show new peaks arising in the HS and splitting of the graphene G peak; these can be considered the first signs of interaction. A small bandgap opening was theoretically predicted for these structures, but the definite experimental proof is still missing, given the high p doping that these HSs show. Electrical measurements with electrolyte gating on the HSs should allow determining the width of the bandgap.

Nr. 36: Narrowband interlayer high-lying excitons in WSe_2 bilayers

Jonas M. Bauer, Sebastian Bange, Kai-Qiang Lin

Transition-metal dichalcogenide (TMDC) semiconductors show a wealth of exciton physics. Here, we present the existence of a new excitonic species, the high-lying exciton (HX), in TMDC monolayer and bilayer with almost twice the band-edge A-exciton energy and with a linewidth as narrow as that of band-edge excitons (Figure 1) [1]. The HX is populated through momentum-selective optical excitation in the K-valleys, and is identified experimentally in upconverted photoluminescence (UPL) and theoretically in ab initio GW-BSE calculations. The coincidence of such high-lying excitonic species at around twice the energy of band-edge excitons explains the efficient exciton-exciton annihilation, and enables the excitonic quantum-interference phenomenon revealed in optical second-harmonic generation (SHG) [2]. The interlayer high-lying excitons in bilayer WSe_2 can be largely tuned by twisting [3] and Stark effect, which gives control over the excitonic quantum interference and the corresponding optical nonlinearity.

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Nr. 37: Mapping of many-body states, orbital texture and interfacial dynamics with (tr)ARPES

S. Beaulieu, T. Pincelli, T. Vasileiadis, S. Dong, J. Maklar, A. Neef, M. Schüler, J. Minar, M. Wolf, L. Rettig, and R. Ernstorfer

Angle-resolved photoemission spectroscopy (ARPES) is the most direct technique for investigating the electronic band structure of crystalline solids. To completely characterize the electronic structure of (topological) materials, one needs to go beyond band structure mapping and probe the orbital texture, associated with Berry curvature and topological invariants. We developed new measurement methodologies in ARPES based on i) crystal rotation mimicking symmetry operations like time inversion or mirror plane reflection and ii) continuous modulation of the ionizing radiation polarization axis.

Such manipulation of the photoemission transition dipole matrix elements together with theory inputs, allows accessing i) the momentum-dependent orbital texture [1-2] and ii) the complex Bloch wavefunction [3], here exemplified for transition metal dichalcogenides - TMDCs. These results represent an important step towards going beyond band structure (eigenvalues) mapping and learn about electronic wavefunction and orbital texture of solids by exploiting matrix element effects in photoemission spectroscopy.

In addition, we extend time- and angle-resolved photoemission spectroscopy (trARPES) [4,5] to study interfacial electron and exciton dynamics in plasmonically van der Waal heterostructures with full momentum-resolution [6].

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Nr. 38: Exciton Landscape in van der Waals Heterostructures

Joakim Hagel, Samuel Brem, Christopher Linderälv, Paul Erhart, Ermin Malic

Van der Waals heterostructures consisting of vertically stacked transition-metal dichalcogenides (TMDs) exhibit a rich landscape of bright and dark intra- and interlayer excitons. In spite of a growing literature in this field of research, the type of excitons dominating optical spectra in different van der Waals heterostructures has not yet been well established. The spectral position of exciton states depends strongly on the strength of hybridization [1] and energy renormalization due to the periodic moiré potential [2]. Combining exciton density matrix formalism and density functional theory, we shed light on the exciton landscape in TMD homo- and heterobilayers at different stackings [3]. This allows us to identify on a microscopic footing the energetically lowest-lying exciton state for each material and stacking. Furthermore, we disentangle the contribution of hybridization and layer polarization-induced alignment shifts of dark and bright excitons, cf. Fig 1. By revealing the exciton landscape in van der Waals heterostructures, our work provides the basis for further studies of the optical, dynamical, and transport properties of this technologically promising class of nanomaterials.

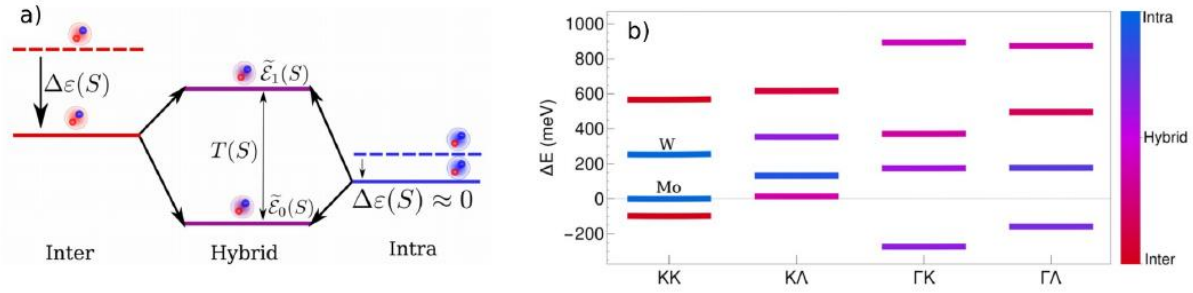

Fig. 1. Schematic for the formation of hybrid excitons. The dashed lines are the unperturbed exciton energies that become shifted due to the layer polarization. Interlayer hybridization results in hybrid exciton states (violet) which are additionally shifted due to avoided crossing. b) Exciton energies for all electron-hole-layer configurations at different valleys with R_h^M stacking.

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