Final workshop of the 1st funding period

March 15 to March 18, 2023

Physikzentrum Bad Honnef

Book of Abstracts

Poster Session A (Thu, 11:30 – 13:00)

Poster Session B (Thu, 16:30 – 18:00)

Poster session C (Fri, 11:30 – 13:00)

List of Posters

A1: Compressive strain in stacked 2D materials: from proximity to metastable hybridization

Bartosz Szczefanowicz[1], Zhao Liu[1], Joao Marcelo J. Lopes[2], Antony George[3], Ziyang Gan[3], Andrey Turchanin[3], Alexander Rothstein[4], Christoph Stampfer[4], and Roland Bennewitz[1]

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2D materials attract much attention for their exotic electronic and mechanical properties. Weak normal-to-plane interactions between layers of 2D materials lead to outstanding tribological properties such as ultralow friction. Friction can be modulated by high contact pressure [1], number of layers [2], application of electric bias [3] and stacking different 2D materials into van der Waals heterostructures [4]. We have performed friction force microscopy (FFM) experiments in ultra-high vacuum to investigate friction on different vdW heterostructures, prepared by different methods (thermal decomposition, chemical vapor deposition, exfoliation). Atomic force microscopy (AFM) and Kelvin probe force microscopy (KPFM) were used for locating and evaluating of heterostructures. Friction forces were determined as function of normal load, of applied electric bias, and of the number of layers. Epitaxial graphene on SiC(0001) undergoes rehybridization into sp^3 under high contact pressure, accompanied by an increase in friction due to formation of covalent bonds with the substrate and the probe [1]. Friction on MoS_2/graphene heterostructures on SiC(0001) depends on the number of MoS_2 layers, which was found to be an effect of changes in adhesion [2]. While almost identical friction was observed for surfaces of hBN and graphene/hBN, it is significantly larger on $MoSe_2$/hBN.

References:

[1] Szczefanowicz, B., et al., Phys. Rev. Res., in press
[2] Liu, Z., et al., Nanoscale, DOI: 10.1039/d3nr00138e
[3] Peng, J. F. et al., Phys. Lett. A, 384, 126166 (2020).
[4] Vazirisereshk, M. R., et al., Nano Lett., 19, 5496 5505 (2019)

A2: Chasing Polaritons: A Pathway to investigate the optoelectronic properties of van der Waals heterostructures

Patryk Kusch and Stephanie Reich

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Our project aims to explore the fundamental physics of interlayer excitons (IE) 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 MoS_2 slabs by imaging their optical near field using scanning type near field optical microscopy. By measuring the dispersion relation of polaritons formed by the *A* and *B* we demonstrate that the exciton-polaritons strongly couple 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 identifying and imaging areas in 2D heterostructures, where interlayer excitons are formed. To that end, we study the influences of excitonic resonances on the local dielectric properties of the TMDs. We used s-SNOM to identify areas of differing dielectric environments and by utilizing a pre-established inversion method we extract the local dielectric function of the sample on the nanometre scale. We succeeded to image by s-SNOM areas on 2D heterostructures that exhibit interlayer excitons. As we are in constant need of high-quality samples, 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 studying electronic and vibronic properties of heterostructures. We observe a red shift in excitonic resonance in the heterostructure when compared to their monolayer counterparts. Finally, in a collaboration with K. Bolotin, we studied free-standing heterostructures and observe propagating interlayer exciton-polaritons and image optically a moiré pattern formed between WSe_2 and $MoSe_2$ layers with a size of 20 nm. By creating double AFM tips together with K. Höflich, we enable in-plane excitation for TERS and s-SNOM experiments, being of huge interest, especially when studying 2D materials.

A3: Interaction effects in graphene/2D polymer heterostructures

Francesca Falorsi[1], Zhiyong Wang[2], Kejun Liu[2], Miroslav Polozij[2], Christian Eckel[1], Thomas Heine[2], Xinliang Feng[2], Renhao Dong[2], Thomas Weitz[1]

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This work explores the interlayer interaction effects of van-der-Walls heterostructures (HS) formed by graphene and a new class of two-dimensional polymers bonded by covalent bonds (C2DPs). These materials can be synthesized with multiple compositions and topology and therefore offer large tunability of their electronic properties.
Via density functional theory calculations, it was possible to predict that coupling of different C2DPs with monolayer graphene should generate new interesting physical phenomena, including band flattening and trivial and non-trivial bandgap opening.
The first system studied is the HSs formed by graphene (either CVD or a mechanically exfoliated) on top of a C2DP that comprises metal-free porphyrin and perylene units linked by imide bonds, in the form of single crystals and monolayers.
Utilizing different techniques we could verify that there are interaction effects in these structures, which depend on the crystallinity of the polymer. In particular, there is a strong mechanical interaction in the hetero-structures formed by single crystals showed by a very defined splitting of the G peak of graphene. The splitting becomes less evident on monolayer samples. All the different types of heterostructures show that the C2DPs p-dopes the graphene; this was confirmed by electrical and KPFM measurements. Finally, ARPES seem to show a change in the band structure of the hetero-structure in respect of the one of graphene.
These promising results indicate that creating C2DP/graphene hetero structures could be a fast and reliable way to engineer the mechanical and electrical properties of graphene.

A4: Non-linear Landau level fan diagram for graphene electrons exposed to a Moiré potential

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The oscillations in the density of states that originate from Landau quantization in a perpendicular magnetic field always produce a fan of linear trajectories in a contour plot of any of the transport quantities in the parameter plane spanned by the density and the magnetic field. This outcome is completely independent of the size of the spectral gaps separating adjacent Landau levels, since only the degeneracy of these levels matters. This degeneracy just depends on the number of flux quanta that pierce the two-dimensional electron system and nothing else. The linear trajectories are described by a simple Diophantine equation of the form $n/n_0 = t\,\varphi/\varphi_0 + s$, where, φ/φ_0 is the normalized flux, and s and t are topological integers representing the band filled at zero field and the quantized Hall conductivity, respectively. This also implies that it is not possible to extract any information about the spectral gaps from such a Wannier diagram, i.e. a density-field diagram. This requires either cyclotron resonance studies or thermal activation experiments. In a van der Waals heterostructure where graphene hosts two-dimensional electrons that are exposed to the Moiré potential of an aligned hBN layer we have discovered conductance oscillations that do not obey this Diophantine equation. The trajectories they describe in a Wannier diagram are non-linear. This anomalous behavior appears only when more than one miniband is occupied and when their Fermi surface areas are different. It can be accounted for by a physical phenomenon referred to as magnetic breakthrough that is a consequence of increasing “uncertainty“ in momentum space. It can be shown that the non-linearity of the trajectories offers the unique opportunity of extracting the level spacings. This technique to extract energy information should be applicable to a broader class of systems such as regularly stacked multilayer graphene (AA, AB, ABC, …) and twisted bilayer graphene.

A5: Spin-orbit coupling-induced correlated phases in rhombohedral trilayer graphene

Yaroslav Zhumagulov, Jaroslav Fabian

No abstract was provided for this contribution.

A6: Light-matter coupling and cavity-QED with moiré excitons in van der Waals heterostructures

Christian Schneider, Stephan Reitzenstein, Christopher Gies

No abstract was provided for this contribution.

A7: withdrawn

A8: Atomistic theory of excited states in van der Waals heterostructures: Moiré confinement strain and electric field effect

Gabriel Bester

No abstract was provided for this contribution.

A9: Excitons in reconstructed moiré heterostructures

S. Zhao, Z. Li, F. Tabataba-Vakili, X. Huang, A. Rupp, J. Göser, I. Bilgin, A. S. Baimuratov, and A. Högele[1]

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Layered transition metal dichalcogenides represent elementary building blocks of van der Waals semiconductor heterostructures. Vertical stacks of monolayers give rise to physical properties that depend sensitively on the choice of materials, the rotation angle between the individual layers, and the emergent band structure. Here, we discuss exciton phenomena in the presence of atomic lattice reconstruction in $MoSe_2$-WSe_2 heterobilayer systems obtained by exfoliation-stacking [1] and chemical vapor deposition [2]. In particular, our experimental studies suggest lattice transformation from ideal moiré periodicity to mesoscopically reconstructed domains for heterostacks near both parallel and antiparallel alignment. We provide a unifying perspective on the origin of the diverse excitonic features associated with mesoscopic lattice reconstruction, and substantiate our findings by one-to-one correlations between observations in optical spectroscopy and secondary electron imaging of the heterostack morphology.

References:

[1] S. Zhao, Z. Li, X. Huang, A. Rupp, J. Göser, I. A. Vovk, S. Yu. Kruchinin, K. Watanabe, T. Taniguchi, I. Bilgin, A. S. Baimuratov, and A. Högele, Excitons in mesoscopically reconstructed moiré heterostructures, arXiv:2202.11139 (2022).

[2] Z. Li, F. Tabataba-Vakili, S. Zhao, A. Rupp, I. Bilgin, Z. Herdegen, B. März, K. Watanabe, T. Taniguchi, G. Schleder, A. S. Baimuratov, E. Kaxiras, K. Müller-Caspary, and A. Högele, Lattice reconstruction in $MoSe_2$-WSe_2 heterobilayers synthesized by chemical vapor deposition, arXiv:2212.07686 (2022).

A10: Many-body theory for quantum gases in moiré-free heterobilayers

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Vertical van der Waals heterobilayers with type-II band alignment such as $MoSe_2/WSe_2$ host layer-separated, Coulomb-correlated electron-hole pairs forming interlayer excitons with binding energies of more than 100 meV and lifetimes that are drastically increased as compared to excitons within a single layer. However, a bosonic gas of excitons undergoes a Mott-type transition to a fermionic electron-hole plasma at sufficiently high electron-hole pair densities. Due to the different physical properties of excitons and fermionic charge carriers, the composition of inter-layer quantum gases has a strong impact on transport coefficients. The diffusion behavior is further influenced by many-body interaction effects within the optically excited quantum gas.

Here, we apply a first-principle theory for moiré-free $MoSe_2/WSe_2$ bilayers based on Wannier functions [1] to describe renormalization effects in fermionic and bosonic inter-layer quantum gases. Using many-body perturbation theory on a GW level, we quantify the density-dependent quasi-particle gap shift, predicting a Mott density of several 10^{12} cm^{-2} depending on temperature. Further, we build on a Hartree-Fock-type description of excitons [2] augmented by dynamical screening to investigate the density dependence of exciton energies. While the well-known dipolar repulsion alone leads to a pronounced blue shift, quantum-mechanical exchange effects as well as phase-space filling and excitonic screening yield renormalization effects of comparable magnitude. Due to strong compensation, a net shift of only a few meV even at exciton densities around 10^{12} cm^{-2} is predicted.

These findings are in excellent agreement with experimental results obtained within our consortium.

References

[1] A. Steinhoff, M. Florian, and F. Jahnke, Physical Review B **104**, 155416 (2021).

[2] V. May, F. Boldt, and K. Henneberger, phys. stat. sol. (b) **129**, 717 (1985).

A11: Tuning and mapping hybrid polaritons at the nanoscale

Hannah Nerl, Katja Höflich

No abstract was provided for this contribution.

A12: Electronic control of spin-orbit and magnetic exchange coupling in graphene-based vdW heterostructures

Lukas Powalla[1], Jonas Kiemle[2], Katharina Nisi[2], Maanwinder Singh[2], Sayooj Satheesh[1], Alexander Holleitner[2], Marko Burghard[1], Christoph Kastl[2]

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Towards the goal of studying SOC proximity effects imparted on graphene, we have explored the optoelectronic properties of Bi_2Te_2Se (BTS)/graphene heterostructures grown by vdW epitaxy. This type of growth ensured a clean and commensurate interface between the two 2D materials, as confirmed by polarization-resolved second-harmonic generation, Raman spectroscopy, and time-resolved magneto-optic Kerr microscopy. Moreover, polarization-resolved photocurrent measurements revealed a circular photogalvanic effect which is drastically enhanced at the Dirac point of the proximitized graphene. This observation is attributed to the gate-tunable, anisotropic interfacial spin structure.

Along similar lines, we have probed the gate-tunable local spin polarisation in current-driven graphene/WTe_2 heterostructures using magneto-optical Kerr microscopy. These measurements revealed that even for a nominal in-plane transport, substantial out-of-plane spin accumulation is induced by a corresponding out-of-plane current flow.

In addition, we have gathered evidence that substitutional doping of the 2D semiconductor WSe_2 by vanadium leads to p-type doping, alongside the emergence of magnetic hysteresis in transport measurements on the V-WSe_2 monolayer both under illumination and without illumination. These findings hint toward the possibility of defect-engineering of the magnetic properties of V-WS_2, albeit the achievable magnetisation is relatively weak.

We furthermore demonstrate the possibility to nucleate individual skyrmions via single nanosecond pulses applied to a vertical nanocontact in exfoliated flakes of the 2D magnet Fe_3GeTe_3 (FGT), implemented into a vdW heterostructure together with an insulating hexagonal boron nitride layer and a graphite top electrode. Additionally, time-resolved scanning transmission X-ray microscopy (STXM) imaging demonstrated the outstanding ability of the nanocontact, while our micromagnetic simulations reproduce the observed skyrmion nucleation process.

A13: Artificial multiferroic van der Waals heterostructures

Stuart Parkin

No abstract was provided for this contribution.

A14: Tuning excitonic quantum optics in stacked van-der-Waals semiconductors

Sebastian Bange

We present published and ongoing efforts in understanding the role of high-lying excitonic species in TMDC materials. High-energy excitonic states first found in monolayer WSe_2 but later confirmed in other TMDC species can be a sensitive probe for interlayer effects due to their narrow, background-free spectra. We review past and ongoing efforts in understanding their excitonic physics and their role in nonlinear wave-mixing and the emergence of quantum interference phenomena such as spectral splitting in second-harmonic generation.

A15: Correlated miniband and multivalley physics in twisted transition metal dichalcogenides

Ursula Wurstbauer

No abstract was provided for this contribution.

A16: Tailoring electronic correlations, excitonics and topological properties in van der Waals heterostructures on ultrafast timescales

Ralph Ernstorfer

No abstract was provided for this contribution.

A17: Optical excitations in transition metal dichalcogenides under pressure

Paul Steeger[1], Jan-Hauke Graalmann[2], Robert Schmidt[1], Philipp Marauhn[2], Marie-Christin Heißenbüttel[2], Jan Nellesen[2], Ilya Kupenko[3], Carmen Sanchez-Valle[3], Steffen Michaelis de Vasconcellos[1], Michael Rohlfing[2], Rudolf Bratschitsch[1]

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One of the most critical parameters in vertical 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. A 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 2H bilayer MoS_2 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 MoS_2 by micromechanical exfoliation and measure stationary optical absorption as a function of pressure using a diamond anvil cell.
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 investigations show a distinct change of the intralayer and interlayer exciton energies, which differ for the A and interlayer exciton. These findings shed light on the fundamental physics of interlayer coupling in 2D semiconductors and have potential implications for the design and optimization of heterostructures for electronic and optical applications.

A18: Straintronics with van der Waals Ferroelectrics

Emeline D. S. Nysten

AG Krenner, Physikalisches Institut, Universität Münster

The emergence of interfacial ferroelectricity in twisted 2D semiconductors has sparked widespread interest in the rapidly developing field of van der Waals materials [1]. This phenomenon has been recently observed in hexagonal BN (hBN) homobilayers [2] as well as in transition metal dichalcogenides (TMDCs) bilayers [3]. This project aims to employ the dynamic strain field of surface acoustic waves (SAWs) to manipulate and sense ferroelectric vdW systems at megahertz to gigahertz frequencies. First preliminary results towards gated ferroelectric vdW stacks on SAW devices obtained within this SPP2244 Seed Funding project are presented. First, TMDC monolayer flakes were successfully heterointegrated onto $LiNbO_3$ SAW devices. Second, key acousto-optoelectric spectroscopy methods are demonstrated using these devices.

References:
[1] C. Wang et al., Nat. Mater. (2023) ; D. Zhang et al., Nat Rev Mater 8, 25-40 (2023)
[2] K. Yasuda et al, Science 372, 1458-1462 (2021) ; M. Vizner Stern et al, Science 372, 1462-1466 (2021) ; C.R. Woods et al, Nat. Commun. 12, 347 (2021)
[3] A. Weston et al, Nat. Nanotechnol. (2022) ; X. Wang et al, Nat. Nanotechnol. (2022)

A19: Spectromicroscopy of 2D interfaces

Niels Schroeter

No abstract was provided for this contribution.

A20: Terahertz nonlinear transport in twisted bilayer graphene and van der Waals heterostructures

L. E. Golub[1], M. Hild[1], M. Otteneder[1], S. Hubmann[1], I. A. Dmitriev[1], G. Di Battista[2], X. Lu[2], D. A. Kozlov[1], K. Watanabe[3], T. Taniguchi[3], D. K. Efetov[2], and S. D. Ganichev[1]

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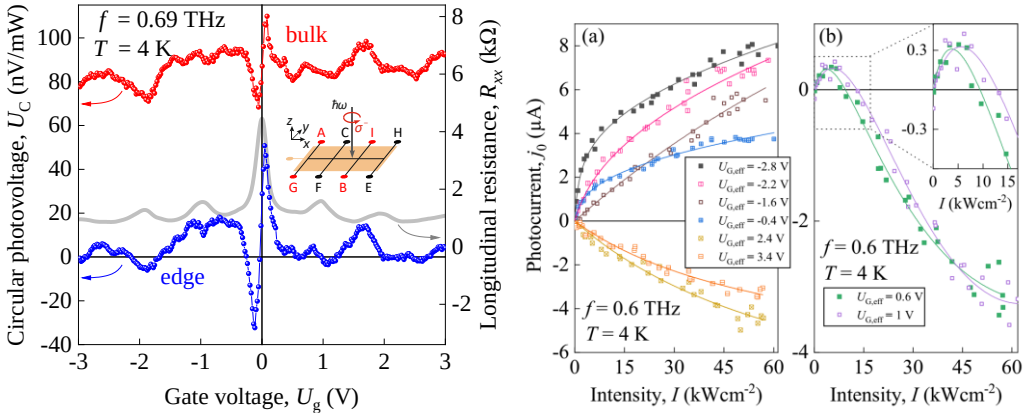
Terahertz excitation of twisted bilayer graphene (tBLG) is shown to result in a photocurrent with direction and magnitude governed by polarization of radiation. We developed a theory describing both linear-polarization dependent and helicity driven photocurrents caused by asymmetrical elastic scattering of photoexcited carriers by tBLG imperfections. The pronounced oscillations upon variation of the gate voltage are registered for both bulk and edge photocurrents [1].
We report on observation of the infrared photoresistance of tBLG under continuous quantum cascade laser illumination. The structure of the photoresponse correlates with weaker features in the dark dc resistance reflecting the complex band structure of tBLG. It is shown that the observed photoresistance is well captured by a bolometric model describing the electron and hole gas heating, which implies an ultrafast thermalization of the photoexcited electron–hole pairs in the whole range of studied temperatures and back gate voltages [2].
Nonlinear intensity dependence of the bulk photogalvanic current and photoconductivity in tBLG is detected. We show that terahertz radiation results in photoresponses, which are caused by indirect optical transitions (free carrier absorption), direct interband transitions, and optical transitions between moiré subbands. We show that the photoresponse saturates at high intensities. For different absorption channels it has different intensity dependencies and saturation intensities. The latter depends nonmonotonically on the Fermi-level position, which is controlled by the gate voltage [3].



Left: Gate voltage dependencies of the bulk and edge circular photovoltages. Right: Dependences of the photocurrent on the radiation intensity for different effective gate voltages.

References:
[1] M. Otteneder, S. Hubmann, X. Lu, D. A. Kozlov, L. E. Golub, K. Watanabe, T. Taniguchi, D. K. Efetov, and S. D. Ganichev, Nano Lett. **20**, 7152 (2020).
[2] S. Hubmann, P. Soul, G. Di Battista, M. Hild, K. Watanabe, T. Taniguchi, D. K. Efetov, and S. D. Ganichev, Phys. Rev. Mat. **6**, 024003 (2022).
[3] S. Hubmann, G. Di Battista, I. A. Dmitriev, K. Watanabe, T. Taniguchi, D.K. Efetov, and S.D. Ganichev, 2D Materials **10**, 015005 (2023).

A21: Microscopic understanding of correlation effects in twisted van der Waals [hetero]structures

Carsten Honerkamp

No abstract was provided for this contribution.

A22: Tunable twistronics: local tuning and probing of topological edge states and superconductivity in bilayer graphene

Christoph Stampfer

No abstract was provided for this contribution.

A23: Integration of Air Sensitive 2D Materials

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A common issue faced when studying 2D materials is their degradation under ambient conditions. This severely hampers their scientific investigation and highlights the importance of encapsulation for their technological application. Superior device characteristics and stability have been achieved using the lithography-free via-contacting scheme. Metal contacts embedded within hexagonal boron nitride (hBN) flakes are used to simultaneously encapsulate devices and electrically contact the 2D material. Encapsulated field effect transistors (FETs) based on indium selenide (InSe) and black phosphorus (BP) demonstrate high quality and stable device operation. InSe FETs demonstrate increased two-terminal mobility of 30-120 $cm^2V^{-1}s^1$ in contrast to just 1 $cm^2V^{-1}s^{-1}$ for their unencapsulated counterparts [1]. Encapsulated BP FETs display superior operation reflected by their higher mobility, lower hysteresis and longterm stability [2].
Additionally, we present our work in the field of all 2D tunnel FETs. Few layer graphene is employed to fabricate devices made entirely of 2D materials. Band-to-band tunneling is demonstrated in tungsten diselenide/ molybdenum disulfide heterojunction transistors with the observation of negative differential resistance confirming the tunneling transport [3].

References:
[1] Arora, H., Jung, Y., Venanzi, T., Watanabe, K., Taniguchi, T., Hübner, R., Schneider, H., Helm, M., Hone, J. C., Erbe, A., ACS Appl. Mater. Interfaces, **11**, 43480-43487 (2019)
[2] Arora, H., Fekri, Z., Vekariya, Y. N., Chava, P., Watanabe, K., Taniguchi, T., Helm, M., Erbe, A., Adv. Mater. Technol., **2200546**, 1-7 (2022)
[3] Chava, P., Watanabe, K., Taniguchi, T., Mikolajick, T., Helm, M., Erbe, A., Device Research Conference (DRC), 978-1-6654-9883-8 (2022)

B1: Skyrmions and Josephson diode effect in 2D materials

Anirban Chakraborty[1], Abhay K. Srivastava[1], Ankit K Sharma[1], Banabir Pal[1], Pranava K. Sivakumar[1], Ajesh Gopi[1], Holger L. Meyerheim[1], and Stuart S.P. Parkin[1]

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Atomically layered materials, held together by weak van der Waals forces, have garnered huge scientific interest ever since the isolation of high quality monolayers of graphene. These class of materials show a wide range of intriguing electrical, magnetic, and optical properties. Here we report on origin of the chiral skyrmions in Fe_3GeTe_2 (FGT) and the Josephson diode effect in Dirac semimetal $NiTe_2$.

The ferromagnetic metal FGT has a significantly high Curie temperature of ~220 K when compared to other 2D magnets. It has been reported earlier that FGT has a centro-symmetric crystal structure. Recently it was shown that Néel skyrmion can be stabilized in FGT as a result of interfacial Dzaloszynski-Moriya interaction (DMI). Using thorough X-ray diffraction analysis, we show that FGT lacks inversion symmetry as a result of asymmetric distribution of Fe vacancies. Furthermore, we confirm the presence of Néel skyrmions using Lorentz TEM. This vacancy-induced breaking of the inversion symmetry of this compound is a surprising new observation and a prerequisite for the bulk type of DMI, rather than interfacial DMI, responsible for the stabilization of Néel-Skyrmion [1].

In a completely different study, we demonstrate a large asymmetry (~80%) in the critical current in Josephson junctions formed from a type–II Dirac semimetal NiTe2 under small magnetic fields (~10 mT). Our experimental data and theoretical analysis suggest that the 'Josephson diode effect' (JDE) is enabled by finite-momentum Cooper pairing in spin-helical topological surface states in an otherwise centrosymmetric system. The finite pairing momentum is further established, and its value determined, from the evolution of the interference pattern under an in-plane magnetic field. The observed giant JDE and a clear understanding of its underlying mechanism paves the way to building novel superconducting devices using Josephson junctions [2].

References:

[1] Chakraborty, A., Srivastava, A.K., Sharma, A.K., Gopi, A.K. et al. Magnetic Skyrmions in a Thickness Tunable 2D Ferromagnet from a Defect Driven Dzyaloshinskii–Moriya Interaction. *Advanced Materials*, **34**, 2108637 (2022)

[2] Pal, B., Chakraborty, A., Sivakumar, P.K. et al. Josephson diode effect from Cooper pair momentum in a topological semimetal. *Nature Physics* **18**, 1228 (2022).

B2: Towards two-dimensional (2D) superconducting spintronics: The "mirage" gap as a signature of triplet superconductivity in an Ising superconductor

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The conventional two-dimensional superconductors are governed by the critical in-plane magnetic field above which the superconductivity is destroyed. Monolayer transition-metal dichalcogenides lack inversion symmetry and along with a strong spin-orbit coupling, lead to valley-dependent Zeeman-like spin splitting. This is the Ising spin-orbit coupling (ISOC) which then lifts the degeneracy of the two valleys and enhances the in-plane critical magnetic field. The finite energy pairings are thus obtained in such systems. The main superconducting gap-like feature shifted to finite energy is observed and termed as “mirage” gap [1]. The triplet correlations are introduced by the applied field, which then affects the critical field of Ising superconductors [2]. The equal-spin triplet pairing is always coupled to the singlet pairing thereby affecting the magnitude of singlet order parameter greatly at higher fields. The density of states (DOS) of the system changes once the triplet order parameter is introduced. The position and importantly the width of the mirage gap is affected by the opposing contributions from the singlet and the triplet order parameter. Thus, the width of the mirage gap can provide one of the signatures of triplet superconductivity in such Ising superconductors.

References:
[1] G. Tang et. al., Phys. Rev. Lett. **126**, 237001 (2021).
[2] M. Kuzmanović et. al., Phys. Rev. B **106**, 184514 (2022).

B3: Improvement and applications of FRG for 2D materials

Jonas B. Hauck, Carsten Honerkamp

Functional renormalization group is a well established method for the study of single-band 2D models. While single-band models still hold open questions, there is an urgent need to broaden the applicability of the method to multi-orbital and multi-site systems. During the SSP2244 funding period we established suitable approximations for this purpose and have put forward an implementation able to handle many models of interest. This enables us to work more closely to real materials, studying their behavior directly inputting Wannier90 data. On this poster, besides introducing the theoretical framework, we will highlight two works of interest; We study the Charge bond ordering in Kagome metals, aiming to give clear observables to decide whether this intricate phase an emergent electronic instability. Beyond this we study an eight-band valley model of twisted bilayer graphene, trying to bridge experimental observations with theoretical predictions.

B4: Compressive strain in stacked 2D materials: from proximity to metastable hybridization

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2D materials attract much attention for their exotic electronic and mechanical properties. Weak normal-to-plane interactions between layers of 2D materials lead to outstanding tribological properties such as ultralow friction. Friction can be modulated by high contact pressure [1], number of layers [2], application of electric bias [3] and stacking different 2D materials into van der Waals heterostructures [4]. We have performed friction force microscopy (FFM) experiments in ultra-high vacuum to investigate friction on different vdW heterostructures, prepared by different methods (thermal decomposition, chemical vapor deposition, exfoliation). Atomic force microscopy (AFM) and Kelvin probe force microscopy (KPFM) were used for locating and evaluating of heterostructures. Friction forces were determined as function of normal load, of applied electric bias, and of the number of layers. Epitaxial graphene on SiC(0001) undergoes rehybridization into sp^3 under high contact pressure, accompanied by an increase in friction due to formation of covalent bonds with the substrate and the probe [1]. Friction on MoS_2/graphene heterostructures on SiC(0001) depends on the number of MoS_2 layers, which was found to be an effect of changes in adhesion [2]. While almost identical friction was observed for surfaces of hBN and graphene/hBN, it is significantly larger on $MoSe_2$/hBN.

References:
[1] Szczefanowicz, B., et al., Phys. Rev. Res., in press
[2] Liu, Z., et al., Nanoscale, DOI: 10.1039/d3nr00138e
[3] Peng, J. F. et al., Phys. Lett. A, 384, 126166 (2020).
[4] Vazirisereshk, M. R., et al., Nano Lett., 19, 5496 5505 (2019)

B5: Effects of atomic reconstructions on correlated states of moiré interlayer excitons

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Correlated states of interlayer excitons (IXs) in a moiré potential are predicted by the Bose-Hubbard model [1]. However, in real systems, atomic reconstructions lead to deviations from the ideal, rigid moiré structure. As a consequence, the moiré potential changes, and with it the effective wave functions of IXs.
In our collaboration, we quantify modifications of the moiré potential and explore in how far atomic reconstruction shifts the boundaries between correlated phases of IXs in the Bose-Hubbard model. We find a non-trivial and twist angle dependent change of the interaction strength and mobility of IXs induced by lattice reconstruction. This effect increases the onsite interaction for large twist angles, pushing the phases of IXs from the supersolid into the Mott-insulating region.

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

B6: Non-linear and negative diffusion of optical excitations in moiré-free heterobilayers

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Vertically stacked heterostructures of transition metal dichalcogenides (TMDCs) present an exciting platform to study electronic many-body phenomena. The type-II band alignments, commonly encountered in TMDC heterobilayers and the presence of strong Coulomb interactions results in the formation of tightly bound and mobile interlayer excitons. What remains barely explored, however, is the high-density regime between excitons and dense plasma in the context of exciton propagation. Moreover, the heterostructures can exhibit substantial complexity due to formation of moiré-type superlattices. It motivates investigation of high-density exciton transport phenomena in the absence of such potentials, to disentangle the effects of dipolar excitons from those stemming from moiré effects. This is the main topic of our study, taking advantage of hBN-encapsulated $WSe_2/MoSe_2$ heterostructures studied in the moiré-free limit of large, atomically reconstructed domains. Using ultrafast microscopy, we show that the interlayer excitons propagate freely even at cryogenic temperatures and low densities. At elevated exciton densities, we demonstrate that in addition to broadly assumed exciton-exciton repulsion, the non-linear increase of the diffusion coefficient also originates from efficient exciton-exciton annihilation. Remarkably, at the exciton ionization threshold of the Mott transition and beyond, we reveal a highly unusual regime of negative effective diffusion that persist for many 100’s of ps after the excitation. This observation presents a particularly interesting case of non-equilibrium phenomena in composite many-particle systems, highlighting the rich physics of optical excitations in van der Waals heterostructures.

B7: Skyrmion formation and multi-spin switching behavior in 2D Van der Waals magnets

Sayooj Satheesh, Lukas Powalla, Max Birch, Kai Litzius, Christoph Kastl, Gisela Schütz, Alexander Holleitner, Marko Burghard

Owing to their atomically flat surfaces and capability to be smoothly integrated into vdW heterostructures, the recent discovery of 2D magnets has opened exiting novel opportunities in the development of 2D spintronic devices with tailored functionalities. Among these, the recently discovered 2D van der Waals (vdW) magnets Fe_3GeTe_2 (FGT, with out-of-plane magnetic anisotropy) and CrSBr (with in in-plane magnetic anisotropy) have attracted particular interest.
We have utilized real-space x-ray (STXM) imaging to determine thickness-dependent magnetic phase diagrams of exfoliated FGT sheets. It turned out that FGT's unique material properties lead to the history-dependent emergence of its magnetic states, i.e., the uniformly magnetized and stripe domain, complemented by a skyrmion-phase-pocket at elevated temperatures. With the help of magnetic simulation, we have identified dipolar interactions as the main stabilisation mechanism for skyrmions.
Furthermore, we have investigated a heterostack consisting of two ribbon-like CrSBr flakes that are rotated by 90° with respect to each other. The magneto-transport properties of this orthogonally-twisted cross-junction device revealed a spin switching behavior which can be explained by the magnetization change along the two in-plane axes of the ribbons.

B8: Theoretical description of moiré excitons in twisted TMD homobilayers

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Multiple monolayers of transition metal dichalcogenides (TMDs) stacked on top of each other are bound via relatively weak van der Waals interactions and thereby offer a rich playground for selective engineering of optical and electronic properties. Even for the case of two identical monolayers forming a homobilayer, we are able to introduce a relative twist angle leading to an emergent superlattice with a large-scale periodicity, that exhibits local modulation of strain and electronic interactions. At the same time, few-layer TMDs feature strongly bound excitons due to reduced dielectric screening in two dimensions. It remains a challenging task to describe such compound particles within the emergent moiré superlattice.
Here, we approach this task by a continuum model based on DFT calculations for an untwisted $MoSe_2$ homobilayer [1]. We extract moiré potentials as well as the corresponding dielectric screening for all dominant high symmetry points of the Brillouin zone and thereby get access to twist angle dependent spectra of different exciton species. We assign the lowest energy state to hybridized interlayer excitons formed between the Γ- and K-valley, exhibiting a strong sensitivity to twist angle, which is in good agreement with experimental results. Furthermore, we predict multiple excitons at higher energies, which are localized at the K-point and show a rather weak angle dependence. Specifically for R-stacking, we find two distinct moiré excitons with dominant intralayer character, while H-stacking yields two degenerate intralayer excitons due to inversion symmetry. In both cases, bright interlayer excitons are found at higher energies.

References:

[1] V. Villafañe, M. Kremser, R. Hübner et al., Physical Review Letters **130**, 026901 (2023).

B9: Probing excitonic population dynamics by nonlinear optical wave mixing in monolayer WSe_2

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Monolayer semiconductors are emerging platforms for strong nonlinear light-matter interaction, due to their giant oscillator strength of tightly bound excitons.

Recently, we reported the existence of a new excitonic species, the high-lying exciton (HX), in monolayer WSe_2. The HX appears at around twice the energy of the band-edge A-exciton, forming a ladder-type excitonic three-level system.

Excitonic quantum interference emerges in second-harmonic generation (SHG) in monolayers[1] and twisted bilayers[2].

Here we apply time-resolved nonlinear spectroscopy to probe the excitonic dynamics in such excitonic three-level system[3]. We find that a significant time difference between two light pulses is necessary for optimal sum-frequency generation (SFG) and four-wave mixing (FWM) when one of the pulses is in resonance with an excitonic transition. The experimental results are explained by numerical calculations based on density-matrix formalism, which provides insights to the coherent exciton dynamics on a femtosecond scale.

Also the influence of a chirped excitation pulse on the quantum interference is presented.

References:

[1] K.-Q. Lin et al., Nat. Phys. **15**, 242-246 (2019).

[2] K.-Q. Lin, J. M. Bauer et al., Nat. Commun. **12**, 1553 (2021).

[3] J. M. Bauer et al., Nat. Photon. **16**, 777 (2022).

B10: Tailored growth of high quality TMD monolayers and their heterostructures

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Chemical vapor deposition (CVD) is considered as one of the most viable routes for scalable growth of transition metal dichalcogenide (TMD) monolayers with tailored properties. Here we present a Knudsen cell based multizone furnace CVD set-up [1], a selection of different TMD monolayers grown with this set-up and their spectroscopic and microscopic characterization down to the nanoscale. We show CVD grown homobilayers with different stacking orders [2], lateral heterostructures of monolayer TMDs with atomically sharp boundaries [3], as well as Janus TMD monolayers with high optical quality [4]. Next, we study the epitaxial growth of MoS_2 and $MoSe_2$ on Au(111) by CVD and MoS_2 by low temperature metal-organic CVD (MOCVD). The properties of these monolayers were characterized by various surface science techniques in ultra-high vacuum including angle-resolved ultraviolet photoelectron spectroscopy (ARUPS), scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) enabling to draw conclusions about their interaction with the substrate.[5] Additionally, we demonstrate that the passivation of SiO_2 substrates with cyclic olefin copolymer significantly improves the performance of TMD monolayers in field-effect devices and photodetectors.[6]

References:

[1] A. George *et al.*: Controlled growth of transition metal dichalcogenide monolayers using Knudsen-type effusion cells for the precursors. *J. Phys. Mater.* **2**, 016001 (2019).
[2] I. Paradisanos *et al.*: Controlling interlayer excitons in MoS_2 layers grown by chemical vapor deposition. *Nat. Commun.* **11**, 2391 (2020).
[3] D. Beret *et al.*: Exciton spectroscopy and unidirectional transport in $MoSe_2$-WSe_2 lateral heterostructures encapsulated in hexagonal boron nitride. *npj 2D Mater. Appl.* **6**, 84 (2022).
[4] Z. Gan *et al.*: Chemical vapor deposition of high-optical-quality large-area monolayer Janus transition metal dichalcogenides. *Adv. Mater.* **34**, 2205226 (2022).
[5] J. Picker *et al.*: Structural and electronic properties of MoS_2 and $MoSe_2$ monolayers grown by chemical vapor deposition on Au(111). Submitted (2023), in corporation with the group of T. Fritz (FSU Jena).
[6] S. B. Kalkan *et al.*: High-performance monolayer MoS_2 field-effect transistors on cyclic olefin copolymer-passivated SiO_2 gate dielectric. *Adv. Optical Mater.* **11**, 2201653 (2023).

B11: withdrawn

B12: Electronic signatures of graphene and hBN implemented in twisted bilayer MoS_2

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Introducing an interlayer twist into bilayer MoS_2 results in the emergence of a moiré structure. When the twist angle θ approaches 0°, a honeycomb superlattice of triangular domains with high-symmetry stacking emerges. This results in the formation of Dirac bands in the electronic band structure as reported by Angeli and MacDonald. [1] In our work, we extend this description to tBL MoS_2 with twist angles both near 0° and 60° using a multiscale approach. Employing a classical force field for structure optimization and density-functional based tight-binding (DFTB), we calculate the electronic structure for systems with up to 5000 atoms and parametrize a tight-binding (TB) model to extrapolate to smaller twist angles with larger moiré cells.

Our results confirm that for $\theta \to 0°$, the honeycomb superlattice of domains with low-energy R_h^M stacking can be associated with the emergence of the Dirac bands. For systems with $\theta \to 60°$, this equivalence between the stacking domains is lifted as they consist of H_h^h and H_h^X stacking with different relative energies. This symmetry break opens a gap in the Dirac bands and can be described by a honeycomb superlattice with different on-site energies. In this way, electronic superstructures resembling graphene and hBN can be implemented into trivial semiconductor MoS_2 by controlling the twist angle. Effective hole masses are found to remain rather light for twist angles down to 1°. In contrast, for twist angles upwards of 58° effective hole masses quickly increase towards infinity. Extrapolation towards twist angles of 0° and 60° thus reveals the formation of flat valence bands.

References:

[1] Angeli, MacDonald, *PNAS*, **2021**, *118*, 2021826118.

B13: Long dark interlayer exciton diffusion length revealed by a CVD-based $MoSe_2/WSe_2$ heterostructure

Andreas Beer[1], Anna Weindl[1], Jacob Fuchs[1], Niclas Maier[1], Antony George[2], T. Taniguchi[3], K. Watanabe[3], Andrey Turchanin[2], and Christian Schüller[1]

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Based on the joint SPP project with the groups of Tobias Korn in Rostock and Andrey Turchanin in Jena we investigate the dynamics of interlayer excitons in CVD-based TMDC heterostructures. In Regensburg, we fabricate heterostructures encapsulated in hexagonal boron nitride from grown $MoSe_2$ and WSe_2 using the so-called hot pickup method. This PDMS-free and dry preparation method allows for a precise angle-dependent fabrication.

CVD materials can exhibit growth-related so-called mirror twin grain boundaries [1], at which the crystal lattice is mirrored by 60 degrees. Therefore, we can fabricate a heterostructure with both 2H- and 3R-stacking and investigate the dynamics of the interlayer excitons in the presence of both stacking orders spectrally and spatially.

References:

[1] A. M. van der Zande, P. Y. Huang, D. A. Chenet, T. C. Berkelbach, Y. You, G.-H. Lee, T. F. Heinz, D. R. Reichman, D. A. Muller and J. C. Hone. *Grains and grain boundaries in highly crystalline monolayer molybdenum disulphide*. Nature Materials **12**, 554–561 (2013).

B14: Proximity-induced topological magnetism

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We explore proximity induced magnetic phenomena combining first-principles approaches and Heisenberg models and account for superconductivity utilising a Bougoliubov-De Gennes formalism. $CrTe_2$ is a particular example that hosts complex magnetism strongly intertwined with its crystal structures [1,2]. We demonstrate that interfacing this 2D layer with various Te-based layers hosting heavy or light elements enables the control of the Dzyaloshinskii-Moriya interaction and magnetic anisotropy energy of the whole heterostructure, and thereby the emergence of new magnetic phases of matter, which are of topological nature such as skyrmions and merons. Also, we found that interfacing graphene with of Co/Au decreases the in-plane magnetic anisotropy energy and in-plane skyrmions exist in Gr/Co/Au without any external field. Finaly, a topological superconductivity was found in $WTe_2/NbSe_2$ vdW heterostructure.

References:

[1] AbuAwwad et al., J. Phys.: Condens. Matter 34, 454001(2022).
[2] Xian et al., Nat. Commun. 13, 257 (2022).

B15: Exciton-Phonon Coupling in $MoSe_2/WSe_2$ Heterobilayers Probed Using Resonant Raman Spectroscopy

Oisín Garrity, Patryk Kusch

Transition Metal Dichalcogenides (TMDs) monolayers can host excitonic states with strong binding energies at room temperature (40 meV to 100 meV [1]) thanks to reduced dielectric screening in monolayer. Upon laying one monolayer on top of another, making a heterostructure, the electronic states of both can hybridise and form a composite structure. Here we use resonant Raman spectroscopy and density functional theory (DFT) to study exciton-phonon coupling of a $MoSe_2/WSe_2$ heterobilayer. Resonant Raman spectroscopy shows an induced resonance in the $MoSe_2$ layer at the A excitonic resonance of WSe_2, while showing no induced resonance in the WSe_2 layer at the A excitonic resonance of $MoSe_2$. Comparing experiment with DFT we show that this induced resonance is a consequence of exciton-phonon coupling, with the induced resonance in WSe_2 being too small to detect. These findings highlight how heterobilayers change upon interaction, and how phonons play an important role in the excitonic properties of these composite systems.

B16: Signatures of superconducting proximity effects in two-dimensional (2D) superconductor/feerromagnet (S/F) bilayers with a helimagnetic metal

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The generation of fully spin-polarised (spin-triplet) Cooper pairs of electrons at the interface of three-dimensional (3D) superconductor/ferromagnet (S/F) has triggered the research field currently known as superconducting spintronics. Several studies have demonstrated that one of the most efficient ways to generate these triplets carrying a net spin in 3D S/F hybrids consists in coupling a S to a F like Ho which has an intrinsic magnetic inhomogeneity due to its helimagnetic spin texture.

Although superconducting spintronics based on 3D S/F thin film multilayers is well-established, the generation of spin-triplet pairs across a van der Waals interface (vdW) has remained an open question. To address this question, we have fabricated van der Waals (vdW) bilayer heterostructures consisting of the two-dimensional (2D) S NbS_2 coupled to the helimagnet $Cr_{1/3}NbS_2$. Performing low-temperature transport studies, we find that the critical temperature (Tc) of these bilayers exhibit an unconventional dependence on the magnetization of the $Cr_{1/3}NbS_2$. We argue, also with the support of a theoretical model, that this behavior demonstrates indirect evidence for generation of spin-triplet pairs at the $Cr_{1/3}NbS_2/NbS_2$ interfaces. Our results set therefore a first milestone towards the application of 2D S/F vdW systems for superconducting spintronics.

References:
[1] J. Linder, J. Robinson, Nat. Phys. 11, 307 (2015).
[2] A. Di Bernardo, S. Diesch, Y. Gu, et al., Nat. Commun. 6, 8053 (2015).
[3] A. Di Bernardo, Z. Salman, X. L. Wang et al., Phys. Rev. X 5, 041021 (2015).

B17: Phonon gap supported tunneling and Faraday screening through graphene

Tobias Wichmann

Encapsulation of van der Waals materials has proven a vital technique to protect them from degradation and contamination. Usually, metallic encapsulation layers mask the properties of the underlying material when studied in scanning tunneling microscopy. Utilizing the inelastic tunneling phonon gap of graphene, however, enables the unfettered investigation of low energy phenomena (e.g. Kondo effect, Majoranas, etc.) by scanning tunneling spectroscopy, while maintaining the advantages of encapsulated samples. Furthermore, we find that the conductive nature of the graphene encapsulation layer screens the sample from tip-induced electric fields, exemplified by our low-temperature STM examination of encapsulated Fe_3GeTe_2.

B18: Theoretical Investigation of 2D-COF/Graphene Multilayer Structures

Shuangjie Zhao, Miroslav Polozij and Thoms Heine

We study the heterostructures and sandwich structures formed by putting covalent organic frameworks (COFs) on graphene to generate superlattice. By performing strain analysis, we found that COFs would break the symmetry of graphene and impose a superlattice onto graphene via the proximity effect, which can alter its electronic properties, such as introducing band gap, doping on graphene ,etc. These results could provide reference and guidance for experimentalists to have expectations and estimations of obtained properties when multi-layer structures are involved.

We use different theoretical methods, including density-functional theory (DFT), DFT based tight-binding and forcefield to perform various types of calculation, such as geometry optimization, band structure calculation, Projected Density of States (PDOS), molecular dynamics ,etc.

B19: Capturing Relaxation Effects and Modelling the Moiré Potentials of Twisted Bilayer TMDs

Carl Emil Mørch Nielsen, Gabriel Bester

In recent years, the research of transition metal dichalcogenides has amassed much attention due to interesting properties such as strong localisation of excited states. The field of twistronics emerged as twisting provides a new degree of freedom in engineering specific properties. However, the theoretical ab-initio approach shows an immediate challenge to overcome; large systems, where the moiré unit cell may hold thousands of atoms.

In this project, the aim is to theoretically study moiré confined optical excitations in twisted transition metal dichalcogenide (TMD) vdW-homo and heterostructures. We have successfully integrated a force-field based method of relaxation using LAMMPS as suggested in a paper by Jain et. al. We have re-parameterized the Stillinger-Weber and Kolmogorov-Crespi potentials seen in this paper and expanded the parameter set to include all possible bilayer TMD combinations. With these we can accurately model the associated local band gap variation, e.g. the moiré potential, taking into effect both lattice corrugation and atomic reconstruction. Our goal is now to investigate the excited state properties with our group-developed code from first-principles.

C1: Interplay between stacking and magnetic configurations in MPS_3 bilayers

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The two-dimensional transition metal thiophosphates MPS_3 (M = Mn, Fe, Ni and Co) have attracted a lot of attention recently because they exhibit a long-range antiferromagnetic (AFM) order and display interesting electronic-optical properties associated with their magnetic state.[1] In these materials, the AFM ground state is governed by the competition between direct M–M exchange and indirect M–S–M superexchange interactions within atomic layers, as well as the d-electron occupancy of the metal ion.[2] However, how the stacking between layers influences the electronic properties of MPS_3 is largely unknown. Here, we perform first-principles calculations to study the interplay between magnetic configurations and different layer stacking in bilayer-MPS_3 systems, cf. Figure 1. Our results provide insight into understanding the AFM configurations in those systems and we suggest that these systems provide a unique playground for studying different aspects of magnetism in 2D systems.

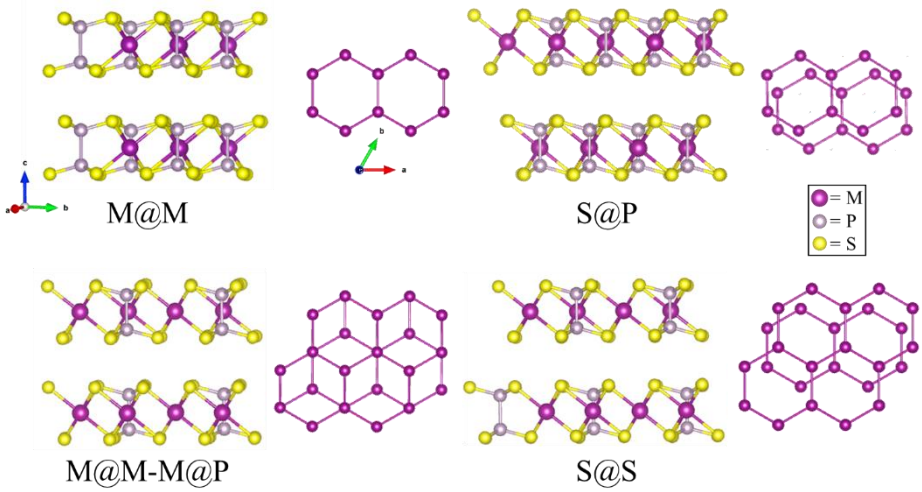

Figure 1. Different high-symmetry stacking configurations in bilayer MPS_3. The top view to the right of each structure indicates the stacking of the two hexagonal lattices of the transition metals.

References:
[1] X. Jiang et al., Applied Physics Reviews, **8** 031305 (2021).
[2] B. L. Chittari et al., Physical Review B, **94** 184428 (2016).

C2: Topological superconductivity and Majorana states in van der Waals heterostructures characterized by scanning probe microscopy

Felix Lüpke

The assembly of van der Waals (vdW) materials into heterostructures enables the engineering of exotic quantum states by interface effects such as moiré and proximity. Scanning tunneling microscopy (STM) has become an important tool to study the properties of such heterostructure, because it gives direct access to the resulting structural and electronic properties. I will give an overview of our results on 1D topological superconductivity in $WTe_2/NbSe_2$ heterostructures, interlayer interactions in twisted bilayer WTe_2 and phonon gap enabled tunneling and interfacial electric fields in graphene/Fe_3GeTe_2 heterostructures.

C3: Critical temperature of superconductor-ferromagnetic bilayers with helimagnetic metals

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Motivated by recent experiments on the proximity effect in superconductor-ferromagnet structures with the helimagnetic ordering of magnetization in the latter, we present a systematic theoretical study of the critical temperature of such systems. By employing the quasiclassical Usadel approach [1], we account for two different configurations of magnetization in the ferromagnet and investigate their impact on the critical temperature (Tc) of the superconductor. Besides recovering the known results for the case of uniform magnetization [2], we find a nontrivial behavior of Tc in the case of spiral magnetization.
Our theory suggests that this can be attributed to the emergence of long-range spin-triplet correlations generated in the ferromagnet [3]. Finally, our model predicts that the presence of spiral magnetization can reduce the critical temperature in the experimentally relevant range of parameters. This effect is the subject of ongoing experiments.

References:
[1] A. I. Buzdin, Rev. Mod. Phys. 77, 935 (2005).
[2] Z. Radović et al, Phys. Rev. B 44, 759 (1991); Ya. V. Fominov et al, Phys. Rev B 66, 014507 (2002).
[3] A. F. Volkov et al, Phys. Rev. B 73, 104412 (2006).

C4: Tailored growth of high quality TMD monolayers and their heterostructures

Julian Picker, Antony George, Ziyang Gan, Christof Neumann, and Andrey Turchanin

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Chemical vapor deposition (CVD) is considered as one of the most viable routes for scalable growth of transition metal dichalcogenide (TMD) monolayers with tailored properties. Here we present a Knudsen cell based multizone furnace CVD set-up [1], a selection of different TMD monolayers grown with this set-up and their spectroscopic and microscopic characterization down to the nanoscale. We show CVD grown homobilayers with different stacking orders [2], lateral heterostructures of monolayer TMDs with atomically sharp boundaries [3], as well as Janus TMD monolayers with high optical quality [4]. Next, we study the epitaxial growth of MoS_2 and $MoSe_2$ on Au(111) by CVD and MoS_2 by low temperature metal-organic CVD (MOCVD). The properties of these monolayers were characterized by various surface science techniques in ultra-high vacuum including angle-resolved ultraviolet photoelectron spectroscopy (ARUPS), scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) enabling to draw conclusions about their interaction with the substrate.[5] Additionally, we demonstrate that the passivation of SiO_2 substrates with cyclic olefin copolymer significantly improves the performance of TMD monolayers in field-effect devices and photodetectors.[6]

References:

[1] A. George *et al.*: Controlled growth of transition metal dichalcogenide monolayers using Knudsen-type effusion cells for the precursors. *J. Phys. Mater.* **2**, 016001 (2019).
[2] I. Paradisanos *et al.*: Controlling interlayer excitons in MoS_2 layers grown by chemical vapor deposition. *Nat. Commun.* **11**, 2391 (2020).
[3] D. Beret *et al.*: Exciton spectroscopy and unidirectional transport in $MoSe_2$-WSe_2 lateral heterostructures encapsulated in hexagonal boron nitride. *npj 2D Mater. Appl.* **6**, 84 (2022).
[4] Z. Gan *et al.*: Chemical vapor deposition of high-optical-quality large-area monolayer Janus transition metal dichalcogenides. *Adv. Mater.* **34**, 2205226 (2022).
[5] J. Picker *et al.*: Structural and electronic properties of MoS_2 and $MoSe_2$ monolayers grown by chemical vapor deposition on Au(111). Submitted (2023), in corporation with the group of T. Fritz (FSU Jena).
[6] S. B. Kalkan *et al.*: High-performance monolayer MoS_2 field-effect transistors on cyclic olefin copolymer-passivated SiO_2 gate dielectric. *Adv. Optical Mater.* **11**, 2201653 (2023).

C5: Interlayer excitons in advanced, CVD-based van der Waals heterostructures with controlled moiré wavelength

Christian Schüller

No abstract was provided for this contribution.

C6: Subnanoscale engineering of 2D magnetism in van der Waals heterostructures

Markus Ternes

No abstract was provided for this contribution.

C7: Robust one-dimensional topological superconductivity in a van der Waals heterostructure probed by Abrikosov vortices

Jose Martinez Castro, Markus Ternes

One-dimensional topological superconductivity is a promising platform for the creation and control of Majorana bound states with potential use for topological quantum computing. To realize the former, proximity-induced superconductivity in quantum spin Hall insulators is a favourable route. Until now, however, confirmation of such an exotic superconducting state has relied on a combination of indirect experimental evidence and theoretical reasoning. Here, we provide direct experimental proof for topological superconductivity in a quantum spin Hall edge state. To this end, we place a monolayer of the quantum spin Hall insulator WTe_2 on the type II s-wave superconductor $NbSe_2$ and use a scanning tunnelling microscope to demonstrate that the induced superconductivity in the quantum spin Hall edge state exhibits a lateral self-proximity effect. This makes the induced superconductivity in the edge state more robust against Cooper pair breaking in the vicinity of an Abrikosov vortex than the two-dimensional proximitized superconductivity in WTe_2. Apart from revealing the distinct topological superconductivity in the quantum spin Hall edge state, our results on a more general note demonstrate the utility of Abrikosov vortices as effective experimental probes for superconductivity in nanostructures.

C8: Superconductor-Ferromagnet van-der-Waals Stacked Devices

S. Singh, M. Klang, P. Ramachandran, O. Millo, N. Bar Gill, A. Di Bernardo, W. Belzig, E. Scheer and H. Steinberg

The recent advent of layered van der Waals (vdW) stacked systems opens a range of new materials which may now be integrated into superconducting devices. vdW materials can be exfoliated down to few layer thickness, allowing the investigation of Superconductor (S) and ferromagnet (F) systems at the 2D limit. To study exfoliated ferromagnets, we developed a NV-center based magnetic imaging technique, where we tracked the evolution of magnetism in the layered magnet Fe_5GeTe_2. To mate S and F flakes, we have developed a stacking method allowing for a clean atomic interface between $NbSe_2$ and Fe_5GeTe_2. Finally, we have studied the tunneling signature of $NbSe_2$ stacked on top of the F insulator $CrGeTe_3$. Our data shows that the S layer becomes sensitive to the magnetization state of the F. Finally, we present a future fabrication technique aimed at integrating diverse materials into a tunnel device.

C9: Other van der Waals platforms and spectroscopy tools for 2D superconducting spintronics

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The extensive range of physical properties of der Waals (vdW) materials and the possibility of stacking them into vdW heterostructures combining their properties paves the way for the realization of devices hosting novel physical phenomena and quantum phases.

We present the results that we have obtained from the investigation of different superconducting Josephson devices based on vdW heterostructures, which host unconventional phenomena including spin-triplet generation and the superconducting diode effect.

We also show a new approach that we have recently developed in our group for the cleaving and exfoliation of nanoflakes from ionic single crystals [1]. These nanoflakes can be used for the fabrication of novel heterostructures where ionic nanoflakes are coupled to conventional vdW materials to extend the range of physical properties and states hosted by such material hybrids.

Last, we report on the development of a low-temperature scanning tunnelling microscope system in our group which is suitable for spectroscopy studies on vdW heterostructures and devices, also in combination with electronic transport.

References:
[1] R. Hartmann, M. Hogen, D. Lignon et al. (Under review).

C10: Interlayer excitons and mode-selective Raman enhancement in hybrid TMDC heterostructures

A. Bergmann, J. Reinhold, M. Hemaid, R. Schwartz, A. George, A. Turchanin, and T. Korn

Most heterobilayer combinations of semiconducting transition metal dichalcogenides (TMDCs) result in a type-II band alignment that drives ultrafast interlayer charge separation. In many cases, the spatially separated carriers can form optically bright interlayer excitons (ILE).

We prepare hybrid TMDC heterostructures by combining mechanically exfoliated and CVD-grown monolayers. This approach can yield multiple heterostructures with a wide range of interlayer twist angles in a single preparation cycle. It is also compatible with full encapsulation of heterostructures in hexagonal Boron Nitride (hBN). We mainly focus on the combination of MoS_2 and WS_2, for which we are able to observe pronounced ILE emission at low temperatures. Additionally, we find a peculiar enhancement of a specific Raman mode of the constituent WS_2 layer in the heterostructures, which is present in both, Stokes and Anti-Stokes spectra. This enhancement can be correlated with the degree of interlayer coupling evidenced by suppression of monolayer exciton emission. Remarkably, it is also observed in WS_2-$MoSe_2$ heterostructures, but absent for the WS_2-WSe_2 material combination.

C11: Spectroscopy in 3R-Transition Metal Dichalcogenides

Swarup Deb, Michael Kempf, Rico Schwartz, and Tobias Korn

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, but so far, most research on rhombohedrally-stacked (3R) TMDs focussed on bilayer units.

Here, we present a systematic study of low-temperature differential reflectivity and time-resolved Kerr rotation in 3R-stacked MoS_2 as a function of stacking configuration, 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 and valley and energy relaxation dynamics on a few-ps timescale.

C12: Subnanoscale engineering of 2D magnetism in van der Waals heterostructures

Samir Lounis

No abstract was provided for this contribution.

C13: Signatures of superconducting proximity effects in two-dimensional (2D) superconductor/ferromagnet (S/F) bilayers with a helimagnetic metal

Angelo Di Bernardo

No abstract was provided for this contribution.

C14: Tunable moiré potentials in 2D-heterostructures using anisotropic strain (TUMPAS-2D)

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We investigate the effect of anisotropic strain on monolayer and heterostructures of transition metal dichalcogenides.

Monolayer transition metal dichalcogenides are ideal for the exploration of spin/valley photo-physics. Here, we investigate the biaxial strain-dependent valley depolarization in monolayer WSe_2 and $MoSe_2$ [1]. We report polarization-resolved photoluminescence measurements on neutral excitons and trions as a function of strain and observe a marked enhancement/diminution of the WSe_2 triplet trion valley polarization with compressive/tensile strain. The origin of this strain-induced effect is shown to be a surprisingly strong strain dependence of the electron-hole exchange interaction, which drives the valley depolarization in these materials. Our experimental findings are in qualitative agreement with ab-inito calculations and rate equation models. The results evidence how strain can be used to tune valley physics in energetically degenerate multi-valley systems.

Large scale two-dimensional moiré superlattices are driving a revolution in designer quantum materials. The electronic interactions in these superlattices, strongly dependent on the periodicity and symmetry of the moiré pattern, critically determine the emergent properties and phase diagrams. To date, the relative twist angle between two layers has been the primary tuning parameter for a given choice of constituent crystals. Here, we establish strain as a powerful mechanism to in-situ modify the moiré periodicity and symmetry [2]. We develop an analytically exact mathematical description for the moiré lattice under arbitrary in-plane heterostrain acting on any bilayer structure. We demonstrate the ability to fine-tune the moiré lattice near critical points, such as the magic angle in bilayer graphene, or fully reconfigure the moiré lattice symmetry beyond that imposed by the unstrained constituent crystals. Due to this unprecedented simultaneous control over the strength of electronic interactions and lattice symmetry, 2D heterostrain provides a powerful platform to engineer, tune, and probe strongly correlated moiré materials.

References:
[1] Z. An, P. Soubelet et al., in preparation (2023)
[2] M. Kögl, P. Soubelet et al., arXiv:2207.12115 (2022), accepted and in press, *npj 2D Mat.*

C15: Proximity-enhanced valley Zeeman splitting at the WS_2/graphene interface

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Van der Waals layered materials allow for the assembly of intentionally designed material stacks or devices with a dedicated topology or functionality. A key concept in this regard is proximity, where an ordered state is transferred from one layer to another region without strongly affecting its electronic structure, even though a direct overlap of the wavefunction in the adjacent layers is required.

In recent years, the interface of graphene with a monolayer transition-metal dichalcogenide (TMD) has received wide attention. This system provides the appealing situation of creating a hetero-junction between a material with strong spin-orbit coupling (SOC of the ML TMD) and long spin lifetimes (graphene). With respect to spin physics, particular interest was given to the topic of proximity-induced spin-orbit coupling in graphene due to the strong SOC of the TMD. On the other hand, graphene has been shown to be a very efficient material for dielectric screening, enabling tunable modification of the exciton binding energy and single particle bandgap. Theoretically, it is expected that the modification of the single particle gap affects the coupling between conduction and valence band, and therefore modifies the exciton valley Zeeman g-factor.

Employing circularly polarized magneto-reflection spectroscopy on large area CVD films of monlayer WS_2 on SiO_2 or single/double encapsulated with monolayer graphene up to 60T, we investigate the valley Zeeman splitting of the A and B-exciton of WS_2 ($X^{A,B}$) [1]. Clear valley Zeeman splittings for the excitons are observed, providing accurate measurements of the valley Zeeman *g*-factors for each sample. While the *g*-factor of X^A varies smoothly and in accord with the shrinking bandgap due to the dielectric environment, the magnetic moment of X^B surprisingly varies stronger in magnitude and distinctly non-monotonically.

We investigate the results with detailed DFT calculations and show that band-folding effects, which originate in commensurate stacking of the van der Waals layers, distinctly affect the lower of the conduction bands of the WS_2 layer, therefore particularly affecting the B-exciton of WS_2.

Our results expand the notion that proximity effects directly affect the admixture of adjacent bands on the wavefunction level. This may lead to resonant coupling effects and therefore shows novel tunability of van der Waals stacks.

References:
[1] Paulo E Faria Junior, Thomas Naimer, Kathleen M McCreary, Berend T Jonker, Jonathan J Finley, Scott A Crooker, Jaroslav Fabian, Andreas V Stier, arXiv:2301.12234 (2023)

C16: Transport Properties of 2d Heterostructures

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The stacking- and folding angle of 2D materials has emerged as an important, novel tuning parameter for the tailoring of optical, mechanical, electronic and magnetic properties. Therefore, it is highly desirable to gather insight into the electronic formation of these structures.

Especially, the electronic properties of twisted bilayer graphene strongly depend on relative orientation of the two atomic lattices [1]. Self-assembled folded graphene structures generated via atomic force microscopy technique [2, 3, 4] shows not only the typical electronic properties of twisted graphene layers but also phenomena due to the folded region [5, 6]. In our magnetotransport measurements, we observe an additional peak, which is independent of the magnetic field. This peak at a certain charge carrier density is attributed to the compressive strain due the folded edge [6].

In the field of 2d semiconductors, the family of transition metal chalcogenides offers a wide range of materials. Among them hafnium pentatelluride ($HfTe_5$) attracts significant interest. Single layers of this material are theoretically predicted to be quantum spin Hall insulators with a large band gap. In conductance-temperature measurements on $HfTe_5$ of different thicknesses, it became clear that the band gap increases with decreasing layer thickness. From this, a band gap of 403 meV was extrapolated for a single layer [7], which corresponds almost exactly to the theoretical prediction.

Also, we investigated thin films of zirconium triselenide ($ZrSe_3$) in reference to their thickness and electrical properties. The material shows a change in band gap energy with thickness from 0.63 eV for a thinner sample to 0.58 eV to a thicker sample. Furthermore, it was possible to see the transistor behavior, showing that the material is an n-type semiconductor [8].

References:

[1] H. Schmidt et al., Nat Commun. **5**, 5742 (2014).
[2] J. C. Rode et al., Ann. Phys. **529**, 1700025 (2017).
[3] J. C. Rode et al., 2D Mater. **6**, 015021 (2018).
[4] L. Bockhorn et al., Appl. Phys. Lett. **118**, 173101 (2021).
[5] S. J. Hong et al., 2D Materials, **8**, 045009 (2021).
[6] S . J. Hong et al., Phys. Rev . B, **105**, 205404 (2022).
[7] C. Belke et al., 2D Mater. 8, 0350292021 (2021).
[8] L. Thole et al., ACS Omega 7, 39913 – 39916, (2022).

C17: Strain is Simple, but Powerful: Case studies of strain engineering in emerging materials

Fei Ding

Even 0.01% strain should not be underestimated in material science. Strain is an important fundamental parameter to (fine-)tune the various properties of materials. However, for many emerging materials, the current strain engineering techniques have limitations:

- Operation at liquid helium temperatures (< 4K). Studying materials at low temperatures has enabled the discovery of many important phenomena. It is however a practical challenge to incorporate strain engineering techniques in low-T experiments.
- Complex/Advanced strain geometry: Uniaxial and biaxial strains are two most common strain geometry in experiments. For crystalline materials, can we apply arbitrary strains?
- Compatibility with high-resolution optics and transport experiments: In these experiments, the materials should not be bended or twisted.
- On-chip integration for real devices: Strain engineering is powerful, however, it is not trivial to perform it on a chip. For practical applications, this is a serious challenge.

Our group has been developing a novel strain tuning technique in the past years. It is based on a piezoelectric ceramic material PMN-PT (0.72 $PbMg_{1/3}Nb_{2/3}O_3$- 0.28 $PbTiO_3$) that can work at cryogenic temperatures. The latest development enables the on-chip integration with quantum photonics and transport platforms. It is a valuable tool for many interesting research directions

C18: Angle-resolved optical spectroscopy of monolayer and heterostructure transition-metal dichalcogenides

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In the past few years, interesting and exotic optical properties of 2D transition-metal dichalcogenides (TMDs) emerged in theoretical considerations and later in pioneering experimental works. Amongst that, the prediction and practical evidence of coexisting light-light and particle-like excitons in monolayer TMDs deserve particular attention due to two facts: Firstly, that even in theoretical works, different ways to treat electronic valleys, interactions and screening seemingly could hide this unusual excitonic feature from discovery. Remaining unnoticed or disregarded in the 2D community for quite a while, the longitudinal ("linear") branch next to the transverse ("parabolic") branch of the else widely examined 2D exciton mode awaited an elevation from the theory and concept level to the domain of experimental revelation, and with it recognition. Induced by hybridization of valleys, the exciton fine-structure with distinct dispersion and polarization properties for finite in-plane momenta was directly evidenced through angle-resolved optical spectroscopy eventually. This comes along the other fact that there lies a challenge in resolving any such dispersion features or splittings in angle-resolving measurements on 2D flakes with light, which demands sufficiently narrow spectral lines and clearly restricts access to *k*-space by the light cone's expanse within a marginal range of center-of-mass momenta, for which the decay of the quasiparticle can result in free-space light output from its 2D plane under momentum conservation. Micro-photoluminescence (μPL) and white-light reflection at cryogenic temperatures finally delivered the clue that an else commonly neglected feature could be detected within accessible collection angles. Similarly interesting and more straight-forward is the direct experimental access to radiation profiles from out-of-plane and in-plane emitters hosted by these popular 2D crystals, such as bright and semi-dark "gray" excitons, respectively. Angle-resolved PL of hBN-encapsulated high-quality TMDs with their multitude of sharp low-temperature lines including dark-exciton phonon sidebands provided insight into the zoo of 2D excitons and their dipole orientations. In this regard, monolayer-monolayer type-II heterostructures gave rise to studies of the emission direction of intralayer and interlayer species (interface-separated electron–hole pairs) in moiré-affected TMD stacks. This presentation highlights foundational experiments in this exciting research direction, to be ultimately carried forward by the 2D community and utilized in future devices.

References:

1) D.Y. Qiu et al., Phys. Rev. Lett. 115 176801 (2015)
2) T. Deilmann & K.S. Thygesen, 2D Mater. 6 035003 (2019)
3) L. M. Schneider et al., Opt. Express 27, 37131 (2019)
4) L. M. Schneider et al., 2D Materials 8, 015009 (2020)
5) L. M. Schneider et al., Sci. Rep. 10, 8091 (2020)
6) M. A. Aly et al., Sci. Rep. 12, 6939 (2022)

C19: Correlated Miniband and Multivalley Physics in Two-Dimensional [Hetero]structures

Gautam Rai, Tim Wehling

No abstract was provided for this contribution.

C20: Superconductivity and Magnetism in ABCB Quadlayer Graphene and biased Bernal Bilayer Graphene

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Recent experiments reported superconductivity in (moiré-less) bi- and trilayer graphene systems. As external magnetic fields and proximity induced spin-orbit coupling are found to stabilize the superconducting order, experiments suggest an exotic spin-triplet order parameter. These findings motivate a theoretical investigation of electronic pairing mechanisms in few-layer graphene systems. This work focuses on a recently observed stacking sequence of quadlayer graphene (“ABCB stacking”) that does not require externel electric fields to gap the bands, as well as biased Bernal bilayer graphene – which also features a band gap and displays a similar Fermi surface.

We use (i) the random phase approximation and (ii) the functional renormalization group to study how short- and long-ranged Coulomb interactions induce spin- and charge-fluctuation driven pairing. The nature of the superconducting order parameter is found to sensitively depend on the interaction strength. Since few-layer graphene systems are susceptible to magnetic instabilities, we argue that the experimentally relevant superconducting instabilities are those driven by spin fluctuations, namely f-wave symmetric pairing states.

C21: Magnetic imaging of skyrmionic spin texture and path toward magnetic two-dimensional material

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In my poster, I will show results of two projects that demonstrate how my current line of research fits the scope of SPP 2244. First, I will introduce the potential of spin-polarized scanning tunneling microscopy being used to characterize non-collinear spin textures in ultrathin magnetic layers on heavy-metal substrate. Second, I will describe new pathways to engineer a transition metal dichalcogenide into a new compositional phase, which allows development of new magnetic two-dimensional materials.

In the first project, we found that double-layer Fe grown on Ir(110) shows an atomic scale spin-spiral, which is stabilized by frustration of exchange interaction and requires enormous fields to unwind it into skyrmions. We demonstrate that it is possible to reversibly weaken the frustration through hydrogen adsorption to an extent, such that the spin texture eventually becomes dominated by Dzyaloshinskii-Moriya interaction and can be decomposed through an external magnetic field into single elliptical skyrmions within a sea of field-aligned spins.

In the second project, we modified niobium disulfide (NbS_2) that was grown by molecular beam epitaxy on graphene/Ir(111) by postgrowth annealing in ultrahigh vacuum with and without providing additional Nb. We found that NbS_2 undergoes a compositional phase transition via covalent growth. The result is a new material with a quintuple layer structure and stoichiometry of Nb_2S_3. Furthermore, we demonstrate that similar compositional phase transition is achieved when Fe is provided. The result in this case is $Fe_{1/3}NbS_2$, which bulk counterpart is known to be magnetic.

C22: t.b.a.

Peter Kratzer

No abstract was provided for this contribution.

C23: Correlated quasiparticles in MoS_2 mirror twin boundaries on graphene

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Highly symmetric grain boundaries such as mirror twin boundaries in semiconducting transition metal dichalcogenides have metallic bands deep in the band gap of the host material. These new states behave as one-dimensional quasiparticles trapped in an insulating matrix. Additional confinement occurs due to the finite length of the grain boundary, enabling the study of strongly correlated, one-dimensional particle in a box states.

We characterized these confined quasiparticles using scanning tunnelling microscopy and spectroscopy at low temperatures and found that their behaviour cannot be described using a non-interacting, free-electron model. Instead, strong Coulomb interaction transforms the states into two distinct quasiparticles carrying spin and charge with different velocities (spin-charge separation) [1]. Furthermore, we could show that these quasiparticles can be shifted with respect to the Fermi level using a non-invasive doping method [2]. These shifts can lead to the situation that the highest confined state below the Fermi energy is filled with a single electron, creating a paradigmatic spin-1/2 state delocalized along the mirror twin boundary. Coupling between this spin and its conducting substrate [graphene on Ir(111)] leads to the formation of a Kondo resonance [3], which shows excellent agreement to numerical renormalization group simulations of the Anderson impurity model.

References:
[1] W. Jolie et al., Phys. Rev. X **9**, 011055 (2019)
[2] C. van Efferen et al., 2D Mater. **9**, 025026 (2022)
[3] C. van Efferen et al., arXiv:2210.09675