TT 49: Graphene and 2D Materials (joint session TT/HL)

Time: Thursday 15:00–18:30 Location: H33

TT 49.1 Thu 15:00 H33

Magnetotransport of the Radial Rashba Spin-Orbit Coupling in Proximitized Graphene — •Wun-Hao Kang[1,2], Ming-Hao Liu[1,2], and Denis Kochan[2,3] — [1]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [2]Center for Quantum Frontiers of Research and Technology (QFort), National Cheng Kung University, Tainan 70101, Taiwan — [3]Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovakia

Graphene-based van der Waals heterostructures take advantage of tailoring spin-orbit coupling (SOC) in the graphene layer by the proximity effect. The proximity effect can be effectively modeled by the tight-binding Hamiltonian involving novel SOC terms[1] and allows for an admixture of the tangential and radial spin-textures[2]. Taking such effective models we perform realistic large-scale magnetotransport calculations–transverse magnetic focusing–and show that there are unique qualitative and quantitative features allowing for an unbiased experimental disentanglement of the conventional Rashba SOC from its novel radial counterpart, called here the radial Rashba SOC. Along with that, we propose a scheme for a direct estimation of the Rashba angle by exploring the magneto response symmetries when swapping an in-plane magnetic field[3].

[1] M. Gmitra et al., Phys. Rev. B 93, 155104 (2016).
[2] K. Zollner et al., Phys. Rev. B 108, 235166 (2023).
[3] W.-H. Kang et al., Phys. Rev. Lett. 133, 216201 (2024).

TT 49.2 Thu 15:15 H33

Nonequilibrium Spin Transport in Graphene Proximitized by WSe_2 — •Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

Spin-orbit coupling (SOC) in graphene is known to be negligibly weak, on the order of 0.1 meV, due to its composed atom, carbon, a light element of atomic number only 6. A decade ago, it was found that the SOC in graphene can be significantly enhanced simply by attaching it to a transition metal dichalcogenide of strong SOC, known as the spin-orbit proximity effect. Our recent theoretical work in collaboration with a transport experiment on graphene proximitized by WSe_2 reported a supporting number for the SOC as strong as 12.6 meV [1]. Inspired by this finding, here I present numerical results on nonequilibrium spin Hall accumulation in graphene/WSe_2 heterostructures based on the Landauer-Keldysh formalism [2]. Combined with the recently discussed radial Rashba SOC [3], nonequilibrium spin precession will be shown, paving an alternative way to realize the Datta-Das spin transistor.

[1] Q.Rao *et al.*, Nat. Commun. **14**, 6124 (2023);
[2] B.K.Nikolic *et al.*, Phys. Rev. Lett. **95**, 046601 (2005);
[3] W.-H.Kang,M.Barth,A.Costa,A.Garcia-Ruiz,A.Mrenca-Kolasinska, M.-H.Liu, D.Kochan, Phys. Rev. Lett. **133**, 216201 (2024).

TT 49.3 Thu 15:30 H33

Resistively Detected Electron Spin Resonance and g Factor in Few-Layer Exfoliated MoS_2 Devices — •Chithra H. Sharma[1,2], Appanna Parvangada[2], Lars Tiemann[2], Kai Rossnagel[1,3], Jens Martin[4], and Robert H. Blick[2,5] — [1]Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [4]Leibniz Institut für Kristallzüchtung, 12489 Berlin, Germany — [5]University of Wisconsin-Madison, University Ave. 1550, Madison, 53706, Wisconsin, USA

MoS_2 has recently emerged as a promising material for enabling quantum devices and spintronic applications. In this context, the demonstration of resistively detected electron spin resonance (RD-ESR) and the determination and improved physical understanding of the g factor are of great importance. However, its application and RD-ESR studies have been limited so far by Schotttky or high-resistance contacts to MoS_2. Here, we exploit naturally n-doped few-layer MoS_2 devices with ohmic tin (Sn) contacts that allow the electrical study of spin phenomena. Resonant excitation of electron spins and resistive detection is a possible path to exploit the spin effects in MoS_2 devices. Using RD-ESR, we determine the g factor of few-layer MoS_2 to be $\approx$1.92 and observe that the g factor value is independent of the charge carrier density within the limits of our measurements.

TT 49.4 Thu 15:45 H33

Unifying Recent Experiments on Spin-Valley Locking in TMDC Quantum Dots — Aakash Shandilya[1], Sundeep Kapila[2], Radha Krishnan[3], Bent Weber[3], and •Bhaskaran Muralidharan[2] — [1]Department of Physics, IIT Bombay, Powai, Mumbai-400076, India — [2]Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India — [3]Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore

The spin-valley qubit promises significantly enhanced spin-valley lifetimes due to strong coupling of the electrons* spin to their momentum (valley) degrees of freedom. Very recently, few experiments on TMDC quantum dots have, for the first time, shared evidence for spin-valley locking at the few-electron limit. Employing quantum transport theory, we numerically simulate the ground- and excited-state transport spectroscopy signatures of these experiments under diverse conditions through a unified theoretical framework, and reveal the operating conditions, based on intrinsic properties, for spin- valley locking. We thus provide a method to experimentally deduce the degree of spin-valley locking based on the SOC strength, inter-valley mixing, and the spin and valley g-factors. Our theoretical analysis provides an important milestone towards the next challenge of experimentally confirming valley-relaxation times using single-shot projective measurements.

[1] A.Shandilya, S.Kapila, R.Krishna, B.Weber B.Muralidharan, ArXiv:2410.21814 (2024).

TT 49.5 Thu 16:00 H33

Estimation of Relaxation Parameters of Spin-Valley Qubits Via Readout Simulations — •Sundeep Kapila, Aparajita Modak, and Bhaskaran Muralidharan — Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India

Two dimensional (2D)-material quantum dot systems, can host multiple qubit possibilities, namely, spin, valley and the spin-valley qubits. The spin-valley qubit, often referred to as the Kramers qubit, is of special interest due to the possibility of long relaxation and coherence times. Experimentally, such long relaxation times (T_1) have been demonstrated in the bilayer graphene (BLG) platform via Elzerman single-shot readout techniques [1-3]. However, there is a lack of comprehensive synergy in explaining the experimental trends in the relaxation times of different types of qubit possibilities, especially at low magnetic fields [1-3]. Here, we present a detailed master equation-based simulation approach to mimic the Elzerman readout schemes to understand the experimental data presented and to characterize the relaxation processes. Our approach allows us to directly extract from the experimental data, the relaxation rates for individual decay processes. We then extend our analysis to unify various experimental data observed across varying conditions in the BLG platform [1-3]. Our analysis backed up by dedicated machine learning algorithms also enables the extension of the model to qubit systems in the transition metal dichalcogenide platform.

[1] Ennslin et al., Arxiv, Mar 2024
[2] Stampfer et al., Arxiv, Feb 2024
[3] Stampfer et al., Nat. Commun. (2022)

TT 49.6 Thu 16:15 H33

Quantum transport in graphene-based Chern mosaics — •Patrick Wittig[1], Fernando Dominguez[1,2], and Patrik Recher[1,3] — [1]Institute of Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Faculty of Physics and Astrophysics and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, 97074 Würzburg, Germany — [3]Laboratory of Emerging Nanometrology, 38106 Braunschweig, Germany

Chern mosaics [1] are systems composed of domains with different Chern numbers within the bulk of the material. Here, the difference in the Chern number between neighboring domains leads to the emergence of chiral boundary modes that propagate along their interface. In our research, we construct a phenomenological scattering network theory based on the symmetries of the system to model the propagation of these chiral modes in triangular and kagome lattice structures, which can arise in graphene-based systems with characteristic valley-chiral edge modes. In particular, we investigate effects such as energy-dependent scattering [2] and spin-orbit coupling [3] within these

networks to analyze the spectrum and transport properties.
[1] S. Grover et al., Nat. Phys. **18**, 885 (2022).
[2] P. Wittig et al., Phys. Rev. B **108**, 085431 (2023).
[3] P. Wittig et al., Phys. Rev. B **109**, 245429 (2024).

TT 49.7 Thu 16:30 H33

Effects of relaxation in deformed graphene structures — Jan Verlage[1], Thomas Stegmann[2], and •Nikodem Szpak[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany — [2]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca, Mexico

It is known that locally deformed graphene creates strong pseudomagnetic fields (of over 100 T) giving rise to Landau levels and being crucial elements of various valleytronic devices. However, taking into account the atomic relaxation of such structures may lead to reduction and regularization of the strain. Here, we revise these effects in various previously studied setups, including membranes and bumps. Our numerical simulations indicate that the atomic relaxation induces a reduction of the pseudomagnetic field by a factor of $5 \div 10$. It may have several consequences for applications.

15 min. break

TT 49.8 Thu 17:00 H33

Landau level mixing in moderately disordered graphene junctions — •Yu-Ting Hsiao and Ming-Hao Liu — Department of Physics,National Cheng Kung University,Tainan 70101,Taiwan

Landau levels are quantized eigenenergy levels in two-dimensional (2D) systems in the presence of an applied perpendicular magnetic field. They are the basic origin of the (integer) quantum Hall effect (QHE). To observe the QHE, i.e., electrical conductance quantized into a sequence of an integer multiple of the universal conductance quantum $\nu * \frac{e^2}{h}$, the sample quality and the strength of the magnetic field typically play the most decisive roles. The cleaner the sample, the weaker the magnetic field required to form the Landau levels. Collaborating with the experiment group led by Prof. Wei Yang from the Institute of Physics(CAS), China, who observed phase shifts of quantized conductance plateaus in ultraclean two-terminal, single-gated graphene devices. From our quantum transport simulations with a systematic tuning of different parameters that could influence the conductance behavior of the graphene device, we found that the experimentally observed phase shift shall arise from the mixing of Landau levels across two neighboring regions with slightly different doping concentrations. Interestingly, we found that the Landau level mixing occurs only when the graphene sample is moderately disordered. In the purely ballistic regime or under strong disorder, the Landau levels mixing fails to form. Our finding reveals a counter-intuitive role played by disorder, possibly also required in other fundamental transport phenomena, such as the Shubnikov-de Haas oscillation.

TT 49.9 Thu 17:15 H33

Dirac meets flat bands: Topological Mottness swap over through hybridization control — Siheon Ryee[1], •Niklas Witt[2,1,3], Lennart Klebl[2,1], Jennifer Cano[4,5], Giorgio Sangiovanni[2], and Tim Wehling[1,3] — [1]Universität Hamburg — [2]JMU Würzburg — [3]Hamburg Centre for Ultrafast Imaging — [4]Stony Brook University — [5]CCQ

Graphene-based multilayer systems provide a versatile platform to explore the interplay between correlation physics and topology. These systems' unique electronic properties arise from their low-energy bands, characterized by significant Berry curvature originating from graphene's Dirac bands, which is believed to play a crucial role in stabilizing emergent correlated states such as superconducting order and various pseudomagnetic states. In this work, we investigate single-site functionalized graphene, where the Dirac bands hybridize with a correlated flat band of localized orbitals. Our findings based on dynamical mean-field theory (DMFT) calculations reveal a hybridization-driven transition between two symmetry-distinct Mott insulators with a protected metallic state emerging in between. Density functional theory (DFT) calculations suggest that the topological transition observed in our model system is achievable in real materials, specifically through the proximity coupling of epitaxial graphene on SiC with group IV intercalants. Unlike phenomena in other correlated graphene-based platforms, such as twisted bilayer graphene and rhombohedral graphene multilayers, the topology-enforced Mottness swap over occurs at a much higher energy scale of electron-volts.

TT 49.10 Thu 17:30 H33

Magnetism in monolayer graphene near 1/4 doping — •Maxime Lucas, Andreas Honecker, and Guy Trambly de Laissardière — Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université / CNRS, France

Recent studies of twisted bilayer graphene (or other 2D materials) have been stimulated by the discovery of correlations between electronic flat-band states due to a moiré pattern [1]. It is shown experimentally and theoretically that the filling of the flat bands affects their magnetic properties significantly. On the other hand, the effect of doping on a simple graphene layer is still unclear. Indeed, its half-filled case is well known [2], but unlike other lattices [3] its magnetic properties beyond half filling are mostly unexplored, except at 1/4 doping [4]. Here, we present our analysis of graphene magnetism using a combination of the Hubbard model and Hartree-Fock mean-field theory. We work at density values around 1/4 doping (average number of electron per site N_e=0.75) as it puts the system right into one of the Van Hove singularities found in graphene's density of states, giving rise to interesting magnetic properties. We present an interaction-density phase diagram and its associated magnetic orders, described by their band structure and spin structure factor.
[1] Y. Cao et al., Nature 556, 43 (2018); Nature 556, 80 (2018).
[2] M. Raczkowski et al., Phys. Rev. B 101, 125103 (2020), and Refs. therein.
[3] R. Scholle et al., Phys. Rev. B 108, 035139 (2023).
[4] S. Jiang, A. Mesaros, Y. Ran, Phys. Rev. X 4, 031040 (2014).

TT 49.11 Thu 17:45 H33

Electronic transport and anti-super-Klein tunneling in few-layer black phosphorus — •Jorge Alfonso Lizarraga Brito[1], Yonatan Bentancur Ocampo[2], and Thomas Stegmann[1] — [1]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca, México — [2]Instituto de Física, Universidad Nacional Autónoma de México, Ciudad de México, México

The electronic transport of few-layer black phosphorus is analyzed theoretically. This work was performed using recent experimental results obtained by μ-ARPES, where tight-binding parameters up to the 4th nearest neighbors within and between the layers were estimated. It is confirmed that the anisotropic band structure of few-layer black phosphorus leads to highly anisotropic transport properties. Most prominently, it is found that the electrons can pass through a potential barrier aligned in a certain crystallographic direction, while for potential barriers rotated by 90 degrees, the transport is completely blocked (anti-super-Klein tunneling). Finally, the study was extended to the case where the top layer of the system is oxidized, showing that the electronic transport is significantly reduced in the oxidized layers, whereas it can be largely unaffected in the central layers.

TT 49.12 Thu 18:00 H33

Pressure-induced structural phase transitions in the van der Waals multiferroic $CuCrP_2S_6$ — •Swarnamayee Mishra[1] and Jochen Geck[1,2] — [1]Institute for Solid State and Materials Physics, TU Dresden, D-01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, D-01062 Dresden, Germany

Two-dimensional (2D) crystals with strong in-plane covalent bonds and weak van der Waals (vdW) interlayer interactions have garnered significant attention following the discovery of graphene and its remarkable properties. $CuCrP_2S_6$ (CCPS) is a promising 2D material exhibiting antiferromagnetic behavior due to the collective ordering of Cr^{3+} spins and antiferroelectric properties driven by Cu+ ion ordering. As a type-I multiferroic, CCPS is particularly notable for its coexistence of antiferroelectricity and antiferromagnetism, coupled with strong polarization-magnetization interactions. These ferroic properties arise from spin-orbit coupling associated with crystal symmetry breaking. Despite its potential, a detailed pressure-dependent crystallographic study of CCPS remains unexplored. In this work, we address this gap using high-pressure single-crystal X-ray diffraction (XRD) to investigate the interplay between structural changes and the material's ferroic behaviors. Our study reveals a phase transition from the low-pressure monoclinic Pc phase to the high-pressure monoclinic C2/c phase at low temperatures, providing new insights into the structure-property relationships of this promising 2D vdW material.

TT 49.13 Thu 18:15 H33

^{31}P NMR studies of quasi-two-dimensional (2D) magnetic correlations in $A\mathbf{CrP_2S_6}$ (A = Cu, Ag) — •Saramgi Sivan[1,2], Kizhake Malayil Ranjith[1], Lukas Prager[1,2], Saicha-

ran Aswartham[1], Bernd Büchner[1,2], and Hans-Joachim Grafe[1] — [1]Leibniz IFW Dresden, D-01069 — [2]Institute for Solid State and Materials Physics, TU Dresden, D-01062

The $AA'P_2S_6$ (A, A' = transition metal ions) family of quasi-2D van der Waals materials has proven to be a model system for low-dimensional magnetism. Here we present detailed ^{31}P NMR measurements on the single crystals of $ACrP_2S_6$. The high-temperature single narrow NMR line shows a splitting at about 160 K for $CuCrP_2S_6$, which is attributed to the antiferroelectric (AFE) transition, while a pake-doublet NMR spectrum is observed for $AgCrP_2S_6$ at room temperature, but no AFE transition at lower temperatures. In $CuCrP_2S_6$, we observed further line splitting below 30 K, reflecting the antiferromagnetic (AFM) order. At $T_N = 30$ K, the NMR spin-lattice relaxation rate $T_1^{-1}(T)$ in $CuCrP_2S_6$ measured at 2.5 T shows a sharp peak due to the critical fluctuations. The T_N is suppressed towards lower temperatures when measured at higher magnetic fields. The $(T_1T)^{-1}(T)$ measured at 7 T shows a broad maximum at about 60 K and a critical enhancement at T_N. On the other hand, $AgCrP_2S_6$ exhibits in-plane AFM order at 20 K, as evidenced by the clear splitting of the NMR spectra, the divergence of $T_1^{-1}(T)$ at T_N, and a broad maximum in the NMR Knight shift. In contrast to $CuCrP_2S_6$, the $(T_1T)^{-1}(T)$ shows only a critical enhancement around T_N without a broad anomaly.