CPP 1: 2D materials and their heterostructures (joint session DS/HL/CPP)

Time: Monday 11:15–13:00 Location: H3

CPP 1.1 Mon 11:15 H3

Tunable phases of Moire excitons in van der Waals heterostructures — •Samuel Brem[1], Christopher Linderälv[2], Paul Erhart[2], and Ermin Malic[1,2] — [1]Philipps University, Marburg, Germany — [2]Chalmers University of Technology, Göteborg, Sweden

Two monolayers of Transition Metal Dichalogenides can be vertically stacked to form a type-II heterostructure, hosting spatially indirect interlayer excitons. Recent studies have shown that moire superlattices can be created by stacking monolayers with a finite twist-angle, giving rise to a tunable modification of exciton features in optical spectra. The moire patterns lead to a spatially varying band gap and consequently, excitons experience a periodic potential modifying their transport properties.

We have combined first-principles calculations with the excitonic density matrix formalism to develop an exciton model for small-angle twisted MoSe2/WSe2 heterostructures. Based on a microscopic approach, we calculate the band structure and wave functions of intra- and interlayer excitons within a twist-tunable moire lattice as well as the resulting optical response. For a range of small twist-angles, we predict completely flat exciton bands corresponding to moire trapped, localized quantum emitters. However, we reveal that this moire exciton phase quickly changes with increasing twist-angle, and at 3°, there are only delocalized excitons. We find the emergence of multiple moire exciton peaks in the absorption, whose spectral shifts with varying twist-angle are characteristic for the trapped or delocalized phase.

CPP 1.2 Mon 11:30 H3

Electrical control of spin-orbit coupling-induced spin precession and spin-to-charge conversion in graphene proximitized by WSe2 — •Franz Herling[1], Josep Ingla-Aynes[1], C. K. Safeer[1], Nerea Ontoso[1], Jaroslav Fabian[2], Luis E. Hueso[1,3], and Felix Casanova[1,3] — [1]CIC nanoGUNE BRTA, Spain — [2]University of Regensburg, Germany — [3]IKERBASQUE, Basque Foundation for Science, Spain

When combined with WSe2, a large spin-orbit coupling gets imprinted by proximity effect into graphene. Here, we use this effect to achieve the strong SOC regime in bilayer graphene. Together with the long, gate tunable spin diffusion, this provides unique control knobs to manipulate coherent spin precession in the absence of an external magnetic field. Remarkably, we observe in these devices that the sign of the precessing spin polarization can be tuned electrically by a back gate voltage and by a drift current. This realization of a spin field-effect transistor at room temperature in a diffusive system, a long-awaited goal of spintronics, could be a cornerstone for the implementation of energy efficient spin-based logic.

In accordance with the large proximity-induced SOC, we also observe spin Hall effect in similar heterostructures with an unprecedented spin-to-charge conversion length of up to 41 nm. Such highly efficient conversion up to room temperature will play a crucial role for the future integration of spintronic devices into existing electronic infrastructure.

CPP 1.3 Mon 11:45 H3

Gate-Switchable Arrays of Quantum Light Emitters in Contacted Monolayer MoS_2 van der Waals Heterodevices — •Alexander Hötger[1,2], Julian Klein[1,2,3,4], Katja Barthelmi[1,3], Lukas Sigl[1,2], Samuel Gyger[5], Takashi Taniguchi[6], Kenji Watanabe[6], Val Zwiller[5], Klaus D. Jöns[5], Ursula Wurstbauer[2,7], Jonathan Finley[1,2,3], and Alexander Holleitner[1,2,3] — [1]Walter Schottky Institut, TU Munich — [2]Exzellenzcluster e-conversion — [3]Munich Center for Quantum Science and Technology — [4]Massachusetts Institute of Technology, Cambridge — [5]KTH Royal Institute of Technology, Dept. of Applied Physics — [6]National Institute for Materials Science, Tsukuba — [7]Institute of Physics, Westfälische Wilhelms-Universität Münster

Controlling single-photon emission on a few nanometers plays an important role for the scalability of future quantum photonic circuits. Moreover, it is highly relevant to facilitate a gate-switchable emission for quantum information schemes. By irradiating MoS_2 with helium ions, we generate single-photon sources at ∼1.75 eV with a lateral position accuracy of only a few nanometers. [1] Second-order correlation measurements unambiguously proof the nature of single-photon emission. Charge doping of the monolayer MoS_2 can be used for switching the quantum emission on and off. [2] This deterministic control of light emission in spatial and temporal means paves the way for new integrated quantum photonic technologies.

[1] J. Klein, L. Sigl et al., ACS Photonics 8, 2 (2021).
[2] A. Hötger et al., Nano Lett. 21, 2 (2021).

CPP 1.4 Mon 12:00 H3

Tunnelling transport in bilayer graphene nanostructures with quantum dots — •Angelika Knothe[1], Vladimir Fal'ko[1], and Leonid Glazman[2] — [1]National Graphene Institute, University of Manchester, Manchester M13 9PL, United Kingdom — [2]Department of Physics, Yale University, New Haven, CT 06520, USA

Quantum nanostructures, e.g., quantum wires and quantum dots, are needed for applications in quantum information processing devices, e.g., transistors or qubits. In gapped bilayer graphene (BLG), one can confine charge carriers electrostatically, inducing smooth confinement potentials while allowing gate-defined control of the confined structure. I will discuss charge transport in BLG nanostructures with electrostatically confined quantum dots. We investigate both theoretically and in collaboration with experiments how the BLG dots' highly degenerate single- and two-electron spin and valley multiplets, which depend on, e.g., the displacement field and the electron-electron interactions, manifest in tunnelling transport. This way, we shed light on BLG material parameters while opening the field for using the dots' rich spin and valley multiplets for quantum information.

1) Theory of tunneling spectra for a few-electron bilayer graphene quantum dot, A. Knothe, L. Glazman, V. Fal'ko, arXiv:2104.03399 2) Probing two-electron multiplets in bilayer graphene quantum dots, S. Möller, L. Banszerus, A. Knothe, L. Glazman, V. Fal'ko, C. Stampfer, et. al, arXiv:2106.08405 3) Quartet states in two-electron quantum dots in bilayer graphene, A. Knothe, V. Fal'ko, PRB 101, 235423 (2020)

CPP 1.5 Mon 12:15 H3

Unconventional Superconductivity in Magic-Angle Twisted Trilayer Graphene — •Ammon Fischer — Institute for Theory of Statistical Physics, RWTH Aachen University

Magic-angle twisted trilayer graphene (MATTG) recently emerged as a highly tunable platform for studying correlated phases of matter, such as correlated insulators and superconductivity. Superconductivity occurs in a range of doping levels that is bounded by van Hove singularities which stimulates the debate of the origin and nature of superconductivity in this material. In this work, we discuss the role of spin-fluctuations arising from atomic-scale correlations in MATTG for the superconducting state. We show that in a phase diagram as function of doping (ν) and temperature, nematic superconducting regions are surrounded by ferromagnetic states and that a superconducting dome with $T_c \approx 2$ K appears between the integer fillings $\nu = -2$ and $\nu = -3$. Applying a perpendicular electric field enhances superconductivity on the electron-doped side which we relate to changes in the spin-fluctuation spectrum. We show that the nematic unconventional superconductivity leads to pronounced signatures in the local density of states detectable by scanning tunneling spectroscopy measurements.

CPP 1.6 Mon 12:30 H3

Twist angle dependent proximity induced spin-orbit coupling in graphene/transition-metal dichalcogenide heterostructures — •Thomas Naimer[1], Klaus Zollner[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Physics, P. J. Šafárik University in Košice, 04001 Košice, Slovakia

We investigate proximity-induced spin-orbit coupling (SOC) in graphene on the four transition-metal dichalcogenides (TMDCs) MoS_2, WS_2, $MoSe_2$ and WSe_2 from first principles. By using different supercells of graphene/TMDC heterostructures we provide systematic insight on the effect of twist angles on the low energy Dirac spectrum. We find that the exact position of the Dirac cone within the TMDC band gap depends linearly on the biaxial strain applied to the graphene. From this relation we extrapolate the zero-strain band offset and correct the band offsets of all calculations by employing a transverse electric field across the heterostructure. The corrected results

reveal massive twist angle tunability of both the magnitude and flavor of proximity induced SOC: We observe a peak in SOC at approximately 19° twist angle and vanishing SOC at 30°. This work was supported by ENB "Topologische Isolatoren" and SFB 1277.

CPP 1.7 Mon 12:45 H3

Predicting the adsorption of alkali metals on 2D materials — Maofeng Dou and •Maria Fyta — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

The adsorption of alkali metal atoms on two-dimensional transition metal dichalcogenides (2D TMDCs) is investigated using quantum-mechanical calculations. Specifically, we evaluate the adsorption characteristics of Li on 2D TMDCs through the respective adsorption energies. We decompose these energies into separate components in order to fundamentally understand the adsorption process. The adsorption energies of lithium on 2D TMDCs were found to strongly and linearly correlate with the energy of the lowest unoccupied states of the materials. Accordingly, we propose and demonstrate the use of this energy as a descriptor for predicting adsorption energies. We further proceed with additional 2D TMDCs and adsorbed alkali atoms in order to generate a database that allows us to learn and make predictions. Our results strongly support the use of the energy of the lowest unoccupied states as a novel efficient descriptor for a data-driven design of materials with pre-selected properties and functions for target applications.