TT 54: Graphene: Electronic structure, excitations, etc. (joint session O/TT)

Time: Wednesday 15:00–17:45 Location: HSZ/0204

TT 54.1 Wed 15:00 HSZ/0204

Magneto-photoelectric effect in graphene via tailored potential landscapes — •Friedemann Queisser[1], Joris Josiek[1,2], Stephan Winnerl[1], and Ralf Schützhold[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

We consider the propagation of charge carriers in planar graphene under the combined influence of a constant transversal magnetic field and an in-plane varying electric potential. By suitably designing the potential landscape, we may effectively steer charge carriers generated by photo-excitation, for example, in order to achieve an efficient charge separation. These finding may pave the way for transport schemes or photoelectric/photovoltaic applications. Funding by the DFG through the SFB 1242 is gratefully acknowledged.

TT 54.2 Wed 15:15 HSZ/0204

Topological obstruction in twisted bilayer graphene — Florie Mesple[1], Pierre Mallet[2], •Guy Trambly de Laissardière[3], Clement Dutreix[4], Gérard Lapertot[5], Jean-Yves Veuillen[2], and Vincent T. Renard[5] — [1]Dept. Physics, Univ. of Washington, Seattle, USA — [2]CNRS, Univ. Grenoble Alpes, Inst. Néel, Grenoble, France — [3]CY Cergy Paris Univ., CNRS, LPTM, Cergy-Pontoise, France — [4]Univ. Bordeaux, CNRS, LOMA, Talence, France — [5]Univ. Grenoble Alpes, CEA, IRIG, PHELIQS, Grenoble, France

The rich physics of magic angle twisted bilayer graphene (TBG) results from the Coulomb interactions of electrons in nearly flat bands of nontrivial topology [1]. Here [2], we perform STM/STS measurements on a moiré pattern generated in a TBG tilted by 4.3°, focusing on a point-like defect. We observe quasi-particle interferences (QPIs) resulting from intravalley backscattering between Dirac cones of graphene layers 1 and 2. Rationalized by tight binding calculations and T-matrix theory, our work shows that the QPIs are strongly impacted by the relative chirality of the Dirac cones of layer 1 and 2 in each valley. It establishes that, within a given moiré valley, the two Dirac cones have the same electronic chirality, as expected in the usual continuum model [3]. This peculiar topology leads to a topological obstruction.

[1] B. A. Bernevig, D. K. Efetov, Physics Today **77**, 38 (2024)
[2] F. Mesple, et al., arXiv:2506.08913 (2025)
[3] R. Bistritzer, A. H. MacDonald, PNAS **108**, 12233 (2011)

TT 54.3 Wed 15:30 HSZ/0204

Quasiparticle Interferences in 30°-twisted graphene quasicrystal — •Jean-Maxime Schlachter[1], Ahmed El Alouani[2], Vincent S Renard[2], Abhishek Karn[1], Ileana Florea[2], Stéphane Vézian[2], Adrien Michon[2], Clemens B Winkelmann[1], and Vincent T Renard[1] — [1]Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, 38000 Grenoble, France — [2]CNRS-CRHEA, Université Côte d'Azur, rue B. Grégory, 06560 Valbonne, France

Quasicrystals are materials that have clean diffraction pattern but no translational symmetry. The advent of van der Waals stacking has opened the possibility to engineer quasicrystals. For example, the moiré pattern in 30°-twisted graphene bilayers has 12-fold rotational symmetry which is not compatible with translation symmetry in 2D, hence it is a quasicrystal (1). Studying this system gives insight into the behavior of Dirac fermions in 2D quasicrystals. ARPES experiments (2) demonstrated the existence of multiple Dirac cone replicas, originating from the incommensurate interlayer coupling. The goal of this study is to determine to what extend these Dirac cone replicas influence the electronic properties of the Dirac fermions. Our low temperature scanning tunneling microscope (STM) experiments evidence the replicated Dirac cones by specific patterns in the local density of states patterns associated with scattering between them, contrary to previous STM experiments (3).

(1) P. Moon et al., Phys. Rev. B, **99**, 16, :165430 (2019) ; (2) S. J. Ahn et al., Science, **361**, 6404, :782-786 (2018) ; (3) C. Yan et al., 2D Mater., **6**, 4, :045041 (2019)

TT 54.4 Wed 15:45 HSZ/0204

Machine Learning for Bandstructure-Structure Relationships in Doped Graphene — •Benedict Saunders[1], Lukas Hörmann[1,2], Valdas Vitartas[1], Chen Qian[1], and Reinhard J Maurer[1,2] — [1]University of Warwick, Coventry, United Kingdom — [2]University of Vienna, Vienna, Austria

The introduction of topological defects or dopants to graphene's honeycomb lattice is a common approach to tuning the electronic and transport properties of the material to suit a specific application. Nitrogen is a widely investigated dopant, which can be introduced into the lattice in various configurations, each with a distinct effect on the material's bandstructure. However, due to the combinatorial explosion of possible dopant configurations, conventional first-principles screening of the electronic bandstructure for all possible configurations is not feasible. Here, we address this limitation by employing the recently developed MACE-H machine learning model to predict the electronic Hamiltonian of nitrogen-doped graphene configurations directly for a series of previously generated defect configurations. This allows us to rapidly generate accurate bandstructures and densities-of-states for large numbers of configurations, enabling the identification of structure-property relationships as a function of temperature and composition.

TT 54.5 Wed 16:00 HSZ/0204

Electronic structure of intercalated epitaxial graphene: A first principles study — •Andres Unigarro[1], Florian Günther[2], and Sibylle Gemming[1] — [1]Institute of physics, TU Chemnitz, Chemnitz, Germany — [2]UNESP, Rio Claro, Brazil

Two-dimensional materials such as graphene are particularly intriguing due to their exceptional mechanical and electronic properties. A natural next step involves combining different 2D materials to form heterostructures with enhanced functionalities. In epitaxial graphene on silicon carbide (SiC), intercalation provides an effective means to tune the electronic, optical, and transport properties of graphene while preserving its honeycomb lattice. Moreover, intercalation enables the synthesis of otherwise unstable 2D layers. In particular, the intercalation of heavy elements such as Pb [1] and Bi [2] is especially promising, as these can introduce strong spin-orbit coupling (SOC) effects [3] (e.g. Rashba effect, gap opening) in graphene. In this work, we use first-principles calculations to investigate the electronic properties of heterostructures formed by Pb and Bi intercalation.

[1] Schölzel, Franziska, et al. ,Small Structures (2024), 2400338
[2] Tilgner, N., et al. Nat Commun 16, (2025), 6171.
[3] Unigarro A., et al. J. Phys. Chem. C (2025), 129, 11, 5617-5624

TT 54.6 Wed 16:15 HSZ/0204

Domain-resolved electronic structure of AgTe-intercalated graphene on SiC(0001): From semiconducting Te-rich interlayer bands to metallic AgTe alloy states — •Vibha Reddy[1], Sawani Datta[1], Bharti Matta[1], Philipp Rosenzweig[2], Ulrich Starke[1], and Kathrin Küster[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, — [2]Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Intercalation at the graphene/SiC(0001) interface provides a powerful route towards engineering the electronic properties of both the graphene and the intercalant. Here, we present the first realization of a transition-metal chalcogen alloy intercalated into the graphene/SiC(0001) interface via AgTe intercalation. The nominally AgTe-intercalated system segregates into multiple microscale intercalation phases, namely, Te-rich, Ag-rich and AgTe alloyed domains. Spatially-resolved and angle-resolved photemission spectroscopy (ARPES) reveals that each domain exhibits distinct graphene doping levels and interlayer band dispersions, highlighting the strong interplay between local intercalation chemistry investigated by X-ray photoelectron spectroscopy (XPS) and electronic band structure. Given the intrinsic spin-orbit coupling and topologically non-trivial states associated with Te- and Ag-based 2D materials, the AgTe alloy-intercalated graphene represents a promising platform for realizing domain-specific emergent quantum phenomena, underscoring the chemical versatility and tunability of alloy-based heterostructures in interface engineering.

TT 54.7 Wed 16:30 HSZ/0204

Proximity-induced electronic states in epitaxial graphene/SiC (0001) via Sn intercalation — •Huu Thoai Ngo[1], Zamin Mamiyev[1], Niklas Witt[2,3], Tim Wehling[2], and

Christoph Tegenkamp[1] — [1]Solid Surface Analysis, Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Institute of Theoretical Physics & Centre for Ultrafast Imaging, University of Hamburg, Hamburg, Germany — [3]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany

Intercalation of heavy elements at the buffer layer/SiC interface is an effective route to decouple it from the substrate while tailoring its electronic properties, for example, energy gap opening [1] and Mott insulating states [2]. In this work, we investigate the Sn-intercalated buffer layer using low-temperature STM/STS, supplemented by SPA-LEED, and DFT calculations. By precisely controlling the intercalation process, we obtain two distinct Sn phases beneath graphene: Sn(1x1) that induces Kekulé-O distortion, and honeycomb-Sn structure that gives rise to Moiré patterns. Remarkably, our STS results reveal a gap opening in Kekulé-O graphene due to Sn-induced sublattice symmetry breaking. In contrast, the honeycomb-Sn phase exhibits Mott insulating states. These findings demonstrate how Sn intercalants modify the structural and electronic properties of graphene at both nano- and microscale. [1] Ghosal, Tegenkamp, C. et al. Phys. Rev. Lett. 129, 116802 (2022). [2] Ghosal, Tegenkamp, C. et al. Phys. Rev. B 111, 235426 (2025).

TT 54.8 Wed 16:45 HSZ/0204

Doping monolayer graphene to the Van Hove singularity — •Guangyao Miao[1], Daniel Jansen[1], Bilal Hawashin[2], Julian Kleeschulte[2], Katharina Offermann[1], Christian Krämer[1], Affan Safeer[1], Abdallah Karaka[1], Jeison Fischer[1], Thomas Michely[1], Michael M. Scherer[2], and Wouter Jolie[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Cologne, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Tuning correlated states in graphene is an intriguing topic, particularly since the experimental realization of superconductivity, correlated insulator states, and magnetic states in twisted-angle bilayer graphene near the magic angle, along with Van Hove singularities (VHSs) tuned to the Fermi level. Such correlated phenomena have also been predicted in monolayer graphene doped to its van Hove singularity. Motivated by this, we study the effect of Cs doping on a graphene monolayer on Ir(111) using MBE. A $\sqrt{3}\times\sqrt{3}$ superstructure is observed due to the Cs intercalations between graphene and Ir(111). Further deposition of Cs on top of graphene leads to the formation of several surface structures with varying Cs concentrations, including adatoms, stripes, and compact islands. Their morphology and electronic structures are revealed by scanning tunneling microscopy and spectroscopy at low temperature. By optimizing the dosage, we successfully tune the VHS to the vicinity of the Fermi level and observe a $2\sqrt{3}\times2\sqrt{3}$ superstructure with respect to the graphene lattice. Possible origins of the superstructure related to many-body interactions will be discussed.

TT 54.9 Wed 17:00 HSZ/0204

Optimizing quantum transport in multi-barrier graphene systems using differential evolution — •Leon Browne and Stephen R. Power — School of Physical Sciences, Dublin City University, Ireland

Potential and mass barriers in graphene introduce electron scattering, modulating transmission probabilities. Complex multi-barrier setups allow electron transmission to be controlled with high precision, but have a huge design space of possible barrier geometries. This work presents a framework to optimize electronic transport in such systems using differential evolution algorithms. First, transfer matrix methods are employed to efficiently compute quantum transport through multi-barrier structures, before optimization is applied to find barrier configurations whose transmission profiles closely match a predefined target profile. To address the trade-off between the accuracy and complexity of resulting barrier configurations, regularization techniques are incorporated into the optimization process. Our approach demonstrates the potential for highly tunable electronic transport in graphene-based systems by exploiting evolution-inspired optimization techniques.

TT 54.10 Wed 17:15 HSZ/0204

Comparative study of plasmons in half-filled graphene via Quantum Monte Carlo and kinetic theory — Maksim Ulybyshev[1], •Adrien Reingruber[1], and Kitinan Pongsangangan[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]Department of Physics, Faculty of Science, Mahidol University, Bangkok

A quantitative description of hydrodynamic electronic transport in strongly correlated materials requires accurate knowledge of collective excitations such as plasmons, which can notably influence viscosity. In free-standing graphene, where long-range interactions are important, standard Dirac-cone perturbation theory misses important finite Brillouin-zone and strong-coupling effects. We investigate plasmons in half-filled free-standing graphene using unbiased Quantum Monte Carlo simulations. Our results reveal well-defined plasmon peaks near the Gamma-point, map their dispersion, and extract the momentum dependence of their quasiparticle residue. Comparing to perturbative predictions, we find substantial deviations arising from the interaction and lattice effects captured only beyond the Dirac approximation. These results underscore the need to incorporate such corrections in analytical theories of electronic transport in graphene.

TT 54.11 Wed 17:30 HSZ/0204

NanoARPES Facility in Shanghai Synchrotron Radiation Facility and Investigation of the Moiré bands in Graphene Devices — •Zhongkai Liu — Shanghaitech University

Spatially resolved angle-resolved photoemission spectroscopy (NanoARPES) is an indispensable tool for probing the electronic structure of exfoliated sample flakes, fabricated devices, and more. In this presentation, we describe the construction, specifications, capabilities, and operation of BL07U-the NanoARPES endstation at the Shanghai Synchrotron Radiation Facility (SSRF) [1]. We will showcase our research on the electronic structure of emerging graphene devices, with a focus on moiré and flat bands. For example, our ARPES studies on magic-angle twisted trilayer graphene clearly reveal the coexistence of moiré flat bands and Dirac bands [2]. In aligned bilayer graphene/hBN heterostructures, we demonstrate that in-situ back gating enables precise tuning of the moiré electronic structure [3]. We directly observe the characteristic topological electronic structures of rhombohedral multilayer graphene, from a 3D generalization of the 1D Su-Schrieffer-Heeger (SSH) chain in thin layers to a topological Dirac nodal spiral semimetal in bulk rhombohedral graphite [4]. Finally, we present our work on the moiré band in bulk alternating twist graphene, which becomes flat at "magic momenta".

Reference: [1] H. Gao et al., Synchrotron Radiation News 37, 12-17 (2024) [2] Y. W. Li et al., Advanced Materials 202205996 (2022) [3] H. B. Xiao et al., Advanced Science 202412609 (2025) [4] H. B. Xiao et al., Science Bulletin 70, 1030-1033 (2025)