TT 4: Graphene, 2D and Twisted Materials

Time: Monday 9:30–12:45 Location: HSZ/0105

TT 4.1 Mon 9:30 HSZ/0105

Toward electron lensing in graphene — Yi-Chen Tsai[1,2], Yu-En Wu[3], Chung-Ting Ke[2,4], and •Ming-Hao Liu[3] — [1]Institute of Physics, Academia Sinica, Taipei, Taiwan — [2]Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan — [3]Department of Physics and Center for Quantum Frontiers of Research and Technology (QFort), National Cheng Kung University, Tainan, Taiwan — [4]Research Center for Critical Issues, Academia Sinica, Tainan, Taiwan

Electron lensing in graphene based on the combined effects of Klein collimation and negative refraction was theoretically proposed in [1]. The proposal promises striking phenomena that could advance the emerging field of electron optics in graphene. Yet, the original design requiring a parabolic pn junction and a point-like injector at the focal point has remained experimentally demanding and unverified. Here, we present recent progress toward realizing electron lensing in state-of-the-art ultraclean graphene devices. These devices feature multiple contacts—point injectors, narrow collectors, and wide drains—engineered to probe the lensing regime. Low-temperature transport measurements are systematically compared with fully ballistic quantum transport simulations at zero temperature. This combined experimental-theoretical approach enables us to assess how closely current devices approach the envisioned lensing regime described in [1] and to identify critical steps still needed for its experimental confirmation.
[1] M.-H. Liu, C. Gorini, and K. Richter, PRL **118**, 066801 (2017).

TT 4.2 Mon 9:45 HSZ/0105

Non-collinear magnetism of flat bands in magic-angle twisted bilayer graphene — •Maxime Lucas[1], Arnaud Ralko[2], Andreas Honecker[1], and Guy Trambly de Laissardière[1] — [1]Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université / CNRS, France — [2]Institut Néel, Université de Grenoble Alpes / CNRS, France

Recent advances of twisted bilayer graphene (and related moiré materials) have been stimulated by the discovery of strong electronic correlations [1] between flat-band states due to a moiré pattern [2]. It is shown experimentally and theoretically that the filling of the flat bands affects their magnetic properties significantly. Similar to what we have done in monolayer graphene [3], we investigate how electronic filling and on-site interactions drive magnetic ordering by studying a Hubbard model on the moiré lattice within an unrestricted Hartree-Fock framework. We mapped out a rich magnetic ground-state phase diagram and uncover a variety of exotic non-collinear spin textures.
[1] Y. Cao et al., Nature 556, 43 (2018); Nature 556, 80 (2018).
[2] G. Trambly de Laissardière et al., Physica E 175, 116362 (2026)
[3] M. Lucas et al., arXiv:2511.22714 [cond-mat.str-el] (2025)

TT 4.3 Mon 10:00 HSZ/0105

Quantum diffusion in twisted bilayer graphene — •Taher Rhouma and Guy Trambly de Laissardière — LPTM, CY Cergy Paris Univ / CNRS, Cergy-Pontoise, France.

The discovery of correlated insulating and superconducting phases arising from the flat bands of magic-angle twisted bilayer graphene (TBG) [1] has stimulated intense interest in their electronic properties. We present a theoretical study of the electronic structure and quantum transport in these flat-band states, incorporating the structural effects of local defects such as non-resonant scatterers. Our real-space method [2,3,4,5] fully accounts for the modification of the electronic structure by defects and for multiple-scattering effects in the conductivity. It shows, in particular, that because of the extremely low Fermi velocity in the flat bands, standard semiclassical Bloch–Boltzmann approaches break down. We present the impact of non-resonant short-range disorder, modeled as diagonal Anderson disorder [4,5] with on-site energies $\varepsilon_i = \varepsilon_0 \pm \Delta W$, on the bandwidth, conductivity, focusing on the impact of filling on the quantum diffusion of twisted bilayer graphene close to the magic angle.
[1] Y. Cao, et al., Nature **556**, 43 (2018); Nature **556**, 80 (2018).
[2] F. Triozon, et al., Phys. Rev. B **65**, 220202, (2002).
[3] O. Faizy Namarvar, et al., Phys. Rev. B **101**, 245407 (2020).
[4] P. Guerrero, et al., Phys. Rev. Lett. **134**, 126301, (2025).
[5] G. Trambly de Laissardière, et al., Physica E **175** 116362 (2026).

TT 4.4 Mon 10:15 HSZ/0105

Quasiparticle Interference as a Probe of Electron's Form Factor in Twisted Bilayer Graphene — D.-H.-Minh Nguyen[1], Francisco Guinea[1,2], and •Dario Bercioux[1,3] — [1]Donostia International Physics Center, 20018 Donostia-San Sebastián, Spain — [2]IMDEA Nanoscience, C/ Faraday 9, 28049 Madrid, Spain — [3]IKERBASQUE, Basque Foundation for Science, Euskadi Plaza, 5, 48009 Bilbao, Spain

We show that characteristics of the electron's form factor in two-dimensional materials are observable in the quasiparticle interference (QPI) spectrum. We study QPI in twisted bilayer graphene using real-space tight-binding calculations combined with the kernel polynomial method, which agrees excellently with the form-factor norm obtained from the continuum Hamiltonian. The QPI signals, displaying a chiral structure, reveal all distinct interference processes between states near the Dirac points. We propose pseudospin textures of twisted bilayer graphene to explain all the interference mechanisms. Our results provide microscopic insights into the electronic eigenstates of twisted bilayer graphene and suggest that QPI could be a promising method for probing the form factor, which governs the material's quantum geometry and many-body states.
[1] D.-H.-M. Nguyen, F. Guinea, D. Bercioux, arXiv:2509.11223.

TT 4.5 Mon 10:30 HSZ/0105

Charge neutrality phase diagram of twisted bilayer graphene from sign-free Monte Carlo simulations — •Johannes S. Hofmann[1], Jong Yeon Lee[2], Patrick Ledwith[3], Eslam Khalaf[4], Ashvin Vishwanath[4], and Erez Berg[5] — [1]Max Planck Institute for the physics of complex systems, Dresden, Germany — [2]University of Illinois at Urbana-Champaign, Urbana, USA — [3]Massachusetts Institute of Technology, Cambridge, USA — [4]Harvard University, Cambridge, USA — [5]Weizmann Institute of Science, Rehovot, Israel

We study the phase diagram of twisted bilayer graphene at charge neutrality as a function of twist angle θ, uniaxial heterostrain ε, and temperature T using sign-problem-free quantum Monte Carlo simulations. At $T = 0$ and zero strain, we find a continuous transition from a Dirac semimetal to a gapped Kramers inter-valley coherent (KIVC) phase as θ decreases toward the magic angle. With finite strain, the KIVC phase undergoes a further continuous transition at smaller θ into an anisotropic semimetal with gapless excitations near the center of the moiré Brillouin zone. In the KIVC regime, the entropy rises sharply with temperature and plateaus at $15\,\mathrm{K} \lesssim T \lesssim 40\,\mathrm{K}$ near the value expected from a Mott-like regime of localized electrons with nearly uncorrelated spin, valley, and orbital degrees of freedom. The spectral function evolves continuously with θ: at low T, a gap opens at the K points and the minimal gap shifts to Γ as θ decreases; at intermediate T, the spectral function smoothly interpolates between a Dirac semimetal spectrum with coherent K-point quasiparticles and a spectrum with gapless Γ-centered quasiparticles near the magic angle.

TT 4.6 Mon 10:45 HSZ/0105

Probing doping profiles in large-angle twisted bilayer graphene by Fabry-Perot interference — •Alina Mrenca-Kolasinska[1], Curtis McDowell[2], Thiti Taychatanapat[2], and Ming-Hao Liu[3] — [1]AGH University of Krakow, Faculty of Physics and Applied Computer Science, Poland — [2]Chulalongkorn University, Department of Physics, Faculty of Science, Patumwan, Bangkok, Thailand — [3]National Cheng Kung University, Department of Physics, Tainan, Taiwan

In graphene, p-n junctions can be induced by electrostatic gating. Fabry-Perot (FP) interferometers formed in gate-defined bipolar cavities have been used to probe Klein tunneling [1], miniband structure in moire superlattices [2], and transport in decoupled bilayer graphene [3]. In this work, we investigate a decoupled large-angle twisted bilayer graphene device that shows rich fringe patterns that resemble FP oscillations. We postulate that they originate from extra electronic cavities created by unintentional local doping in the device. Our quantum transport simulations incorporating this assumption reproduce the observed patterns. Our findings demonstrate that disorder can lead to unexpected and rich structures that can be probed by transport.
[1] A.F. Young, P. Kim, Nat. Phys. 5 (2009) 222.
[2] C. Handschin et al. , Nano Lett. 17 (2017) 328.

[3] P. Rickhaus et al. , Sci. Adv. 6 (2020) eaay8409.

15 min. break

TT 4.7 Mon 11:15 HSZ/0105

Theory for optical control of correlated states in moiré transition metal dichalcogenide heterostructures — •Haoyang Tian and Urban F.P. Seifert — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77a, 50937 Köln, Germany

In recent years, moiré transition metal dichalcogenide (TMD) heterostructures have emerged as highly versatile platforms for investigating phases and phenomena of strongly correlated electrons on emergent lattice scales. However, experimental characterization of the precise nature of some interaction-driven orders, in particular antiferromagnetism, and their excitations has remained a challenge. Given strong light-matter couplings and valley selection rules in TMD materials, ultrafast optical methods may constitute a promising avenue for probing and controlling these states and their collective modes.

In this work, we develop a theoretical framework to describe the coherent light-driven dynamics of type-II moiré TMD heterobilayers under circularly polarized laser irradiation. We construct a moiré-Floquet Hamiltonian for the electronic states under periodic driving. In the off-resonant regime, we find that the moiré valence band flattens due to hybridization with the photon-dressed conduction band and derive an effective low-energy model for the Floquet valence band. By incorporating electron-electron interactions via a Hartree-Fock framework, we analyze the impact of optical driving on the phase structure and collective excitations (e.g., magnons).

TT 4.8 Mon 11:30 HSZ/0105

Unveiling structural transitions in the van der Waals multiferroic $CuCrP_2S_6$ under pressure and temperature — •Swarnamayee Mishra[1,3], Gaston Garbarino[2], Alexander Mistonov[1,3], Steven Gebel[1], and Jochen Geck[1,3] — [1]Institute for Solid State and Materials Physics, TU Dresden, Dresden, Germany — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, Dresden, Germany

Two-dimensional (2D) crystals with strong in-plane covalent bonds and weak van der Waals 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 Cr3+ spins and antiferroelectric properties driven by Cu+ ion ordering. 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, high-resolution single crystal x-ray diffraction is employed to explore its response to variations in pressure and temperature. Our measurements reveal a clear pressure-driven change of lattice symmetry at low temperatures from monoclinic Pc to monoclinic C2/c, together with signatures of charge ordering that point to strong coupling between structure and electronic degrees of freedom. In addition, a pressure-induced reorientation of a structural modulation is found, shifting it from the ac plane at low pressure to the ab plane at higher pressure.

TT 4.9 Mon 11:45 HSZ/0105

Switching Magnetic Anisotropy by Chemical Substitution in Single Crystals of the 2D van der Waals System $(Fe_{1-x}Ni_x)_2P_2S_6$ — •Yuliia Shemerliuk[1], Anja U. B. Wolter[1], Bernd Büchner[1,2], and Saicharan Aswartham[3] — [1]The Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Institute for Solid State and Materials Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, Germany — [3]International Center for Interfacing Magnetism and Superconductivity with Topological Matter - MagTop, Institute of Physics, Polish Academy of Sciences: Warsaw, Poland

During recent years, layered quasi-two-dimensional van der Waals materials have attracted considerable attention in fundamental science due to their intrinsic low-dimensional crystal structure, which affects their physical properties. Among these materials, layered thiophosphates $M_2P_2S_6$ (M= Ni, Co, Fe, Mn, V) stand out as a versatile platform for exploring the interplay between structure and magnetic exchange interactions. In this talk, we will show how chemical substitution and structural tuning influence magnetic ground states in the quasi-2D system $(Fe_{1-x}Ni_x)_2P_2S_6$. This series combines two structurally compatible parent compounds with fundamentally different magnetic behaviors, interlayer couplings, and ordering temperatures. Our magnetization measurements on single crystals across the substitution series reveal antiferromagnetic ground states throughout. Importantly, we observe a continuous reorientation of magnetic anisotropy from out-of-plane to in-plane with increasing Ni content.

TT 4.10 Mon 12:00 HSZ/0105

Tuning surface resonance states on black phosphorus — •Dongming Zhao[1], Byeongin Lee[2], Junho Bang[2], Claudia Felser[1], Jian-Feng Ge[1], and Doohee Cho[2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea

Surface resonance states can significantly alter how semiconductors respond to external electric fields. When present, such states can accommodate charge accumulation at the surface, reducing the response from bulk carriers and thereby suppressing band bending. In this work, we show that surface-resonance states near the band edge of black phosphorus couple strongly to the tip-induced electrostatic potential in scanning tunneling spectroscopy. This coupling produces a characteristic dip in the tunneling conductance spectrum. Our simulations indicate that this dip arises from a field-driven change in the tunneling probability into surface resonance states. By effectively tuning the electric field in the junction, we drive the surface-resonance band across the Fermi level, enhancing its contribution to the tunneling current. Our results illustrate how localized surface resonances under an external field dominate electrostatic screening, highlighting their importance in designing and operating semiconductor devices.

TT 4.11 Mon 12:15 HSZ/0105

Quantifying Twist Angles in Cuprate Heterostructures with Anisotropic Raman Signatures — •Flavia Lo Sardo[1,2], Marina Esposito[3,4], Tommaso Confalone[1,5], Kornelius Nielsch[1,2,5], Nicola Poccia[1,3], and Haider Golam[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden (IFWDresden), 01069 Dresden, Germany — [2]Institute of Materials ScienceTechnische Universität DresdenDresden 01062, Germany — [3]Department of PhysicsUniversity of Naples Federico IINaples 80126, Italy — [4]National Institute for Nuclear Physics (INFN) - Sezione di NapoliNaples 80126, Italy — [5]Institute of Applied PhysicsTechnische Universität Dresden, 01062 Dresden, Germany

Artificially engineered twisted van der Waals (vdW) heterostructures have unlocked new pathways for exploring emergent quantum phenomena and strongly correlated electronic states. Many of these phenomena are highly sensitive to the twist angle, which can be deliberately tuned to tailor the interlayer interactions which makes the twist angle a critical tunable parameter. In particular, twisted cuprate heterostructures based on $Bi_2Sr_2CaCu_2O_{8+x}$ (BSCCO) have demonstrated angle-dependent superconducting properties, positioning the twist angle as a key tunable parameter. In this work, a fully non-invasive, polarization-resolved Raman spectroscopy approach is introduced for determining twist angles in artificially stacked BSCCO heterostructures. By analyzing twist-dependent anisotropic vibrational Raman modes, clear optical fingerprints of the rotational misalignment between cuprate layers are identified.

TT 4.12 Mon 12:30 HSZ/0105

Polaritonic near-field effects on the metal-to-insulator transition of the Hubbard model — •Paul Fadler[1], Marios Michael[2], Katharina Lenk[3], Michael Sentef[1], and Martin Eckstein[3] — [1]Institute for Theoretical Physics, University of Bremen — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [3]Department of Physics, University of Hamburg

The influence of the dielectric environment on material properties has been studied theoretically mostly within two different contexts: Within Coulomb engineering one uses electrostatic screening of the longitudinal electromagnetic field to renormalize interactions [1]. In contrast, within cavity material engineering one tries to shape the transverse electromagnetic field to produce desired material properties [2]. For certain settings, such as in the near-field of materials hosting phonon- or plasmon-polaritons, this separation is no longer possible as the longitudinal and transverse components of the electromagnetic field mix. We investigate the resulting effect on the metal-to-insulator phase transition of a 2-D Hubbard model suspended above a polariton-hosting material using DMFT + GW treating the longitudinal and transverse fields consistently. Lastly, we consider the gauge dependence intro-

duced by our scheme for the Coulomb [3] and Weyl gauge [4].

[1] E. van Loon et al., npj 2D Mater. Appl. **7**, 47 (2023)
[2] F. Schlawin et al., Appl. Phys. Rev. **9**, 011312 (2022)
[3] K. Lenk et al., Phys. Rev. B **106**, 245124 (2022)
[4] C. Eckhardt et al., Phys. Rev. Lett. **135**, 156902 (2025)