TT 84: 2D Materials: Electronic structure, excitations, etc. III (joint session O/HL/TT)

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

TT 84.1 Thu 15:00 HSZ/0204

Linearized augmented plane waves for low-dimensional materials — •Andris Gulans, Ernests Jansons, and Janis Uzulis — University of Latvia, Riga, Latvia

We address the challenge of efficient yet highly precise density-functional theory calculations of low-dimensional materials and present a set of tools and algorithms specific to linearized augmented plane waves (LAPW) that is implemented in the electronic-structure code `exciting`. First, we discuss our iterative eigensolver compatible with local and hybrid functionals. It is an extension of Davidson*s algorithm and does not require explicit Hamiltonian construction while overcoming difficulties associated with high condition numbers. The second important ingredient is the adaptively compressed exchange that represents the non-local (screened) Fock exchange via a low-rank approximation. This approach enables computational complexity as low as $O(N^3 \log N)$ floating-point operations (FLOPs) with N being the number of atoms. It is a novel feature in hybrid functional calculations using LAPW as the standard approaches require $O(N^4)$ FLOPs. Finally, we introduce a cylindrical cutoff for the Coulomb interaction for handling the $q = 0$ singularity.

TT 84.2 Thu 15:15 HSZ/0204

Graphene-Enabled Mott–Metal Transition in Silicon Dangling Bonds — •Niclas Tilgner[1], Siheon Ryee[2], Zamin Mamiyev[1], Philip Schädlich[1], Christoph Tegenkamp[1], Tim O. Wehling[2], and Thomas Seyller[1] — [1]Institute of Physics, Chemnitz University of Technology, Germany — [2]I. Institute of Theoretical Physics, University of Hamburg, Germany

Controlling emergent electronic phases in materials with strong Coulomb interactions remains a central challenge in condensed matter physics. Adatom lattices on semiconducting surfaces provide prototypical platforms for exploring such correlated phenomena. Recent advances have facilitated the synthesis of 2D Mott insulators in proximity to graphene (N. Tilgner et al 2025 2D Mater. 12 045022). Here, we demonstrate that alkali adsorption on a graphene/Si/SiC(0001) heterostructure – where the Si layer hosts correlated dangling bonds – enables controlled charge transfer to the Mott insulator. Beyond a critical carrier concentration, we observe a sudden collapse of the Mott gap, indicating a transition to a correlated metallic phase. Our results point to a finite proximity coupling between the Mott layer and graphene, as recently suggested by a theoretical study (N. Witt et al 2025 arXiv:2503.03700), which gives rise to nonlocal dynamical screening beyond simple electrostatics and provides a natural pathway for the observed phase transition.

TT 84.3 Thu 15:30 HSZ/0204

From self-consistent DFT+DMFT to the two-particle level: Magnetic phase diagram of X:SiC(111) — •Lukas Bongardt[1,2], Niklas Enderlein[3], Giorgio Sangiovanni[4], Philipp Hansmann[3,5], and Henri Menke[1] — [1]Max Planck Computing and Data Facility — [2]Technical University of Munich — [3]FAU Erlangen — [4]Universität Würzburg — [5]University of Iceland, Reykjavík

Recently we have proposed a novel and versatile platform to realize a two-band Hubbard model with massless Dirac fermions and flat bands hosting strong correlations by depositing three different species of transition-metal adatoms on semiconductor surfaces (arXiv:2410.17165). Using state-of-the-art DFT+DMFT calculations we investigated the spectral properties of X:3C-SiC(111) (X = Ti, V, Cr). Due to the presence of well-defined Dirac cones and flat bands, indicating the potential for realizing topological and correlated phases, we identify transition-metal adatoms on SiC as a possible platform for exploring the interplay of correlations, topology, and magnetism in two-dimensional materials.

In this work, we explore the magnetic phase diagram of these systems within DMFT by calculating the generalized two-particle vertex and using it to solve the Bethe-Salpeter equation for the generalized susceptibility. This gives us a fully orbital-, spin-, and most importantly momentum-dependent susceptibility which carries the information about the ordering wave vector and is experimentally accessible through various techniques.

TT 84.4 Thu 15:45 HSZ/0204

Cr 3*d* Orbital Hybridization and Electronic Structure in the Layered Magnetic Semiconductor $CrPS_4$ — •Lasse Sternemann[1], David Maximilian Janas[1], Richard Leven[1], Eshan Banerjee[2], Jonah Elias Nitschke[1], Marco Marino[1], Leon Becker[3], Ahmet Can Ademoglu[1], Frithjof Anders[1], Stefan Tappertzhofen[3], and Mirko Cinchetti[1] — [1]TU Dortmund University, Department of Physics, 44227 Dortmund, Germany — [2]Department of Materials, Imperial College London, London, SW7 2AZ, United Kingdom — [3]TU Dortmund University, Department of Electrical Engineering and Information Technology, 44227 Dortmund, Germany

Despite its promising spintronic and magneto-optical characteristics, the electronic band structure of the van der Waals magnetic semiconductor $CrPS_4$ is still unknown. Here, we report angle-resolved photoemission spectroscopy measurements of its band structure in the para- and antiferromagnetic phase, complemented by DFT+U calculations. Theoretical results reveal dominating Cr 3*d* and S 3*p* contributions to the valence band and a ligand-to-metal charge-transfer band gap. Crystal field split Cr 3*d* orbitals display distinct hybridization regimes with S 3*p* orbitals: t_{2g} orbitals are only weakly affected by hybridization, while e_g states experience a 4 eV anti-bonding/bonding splitting with S-mixing relaxing dipole selection rules, otherwise darkening optical *d*-*d* transitions. These findings establish the ground state electronic and orbital structure of $CrPS_4$ and provide essential benchmarks for understanding its optical and magnetic responses.

TT 84.5 Thu 16:00 HSZ/0204

Spectroscopic Investigation of the Ni Valence States in $NiTe_2$ — •Tassaphon Tirasutt[1], Sheng-Huai Chen[1], Alexander C. Komarek[1], Chun-Fu Chang[1], Yu-Chieh Ku[2], Po-Yu Cho[3], Chun Sum Brian Pang[4], Mizuki Furo[5], Naoki Ito[5], Ulrich Burkhardt[1], Simone G. Altendorf[1], Atsushi Hariki[5], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Yang Ming Chiao Tung University, Hsinchu, Taiwan — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [4]The University of British Columbia, Vancouver, Canada — [5]Osaka Metropolitan University, Osaka, Japan

Nickel-based transition metal compounds exhibit a wide range of properties arising from the strongly correlated *d* electrons. In this study, we investigate $NiTe_2$, a layered transition-metal dichalcogenide with reported type-II Dirac semimetallic properties. While its topological nature has been the focus of interest, the fundamental question of the properties of the Ni ions in $NiTe_2$ has rarely been discussed. We address this issue using soft X-ray core-level and valence-band photoelectron spectroscopy, as well as Ni-$L_{2,3}$ absorption spectroscopy, combined with a theoretical approach using LDA+DMFT. Our findings provide insights into the Ni 3*d* occupation and degree of correlation of the Ni in a metallic ligand bath of the $NiTe_2$ system.

TT 84.6 Thu 16:15 HSZ/0204

TMDC surfaces as scattering targets in spin-polarization detectors: A case study of MoS_2 — •Christoph Angrick[1], Annika Henriksen[1], Nicole Edossa[1], Andre Reimann[1], Moritz Ewert[2,3], Lars Buss[2,3], Jens Falta[3], Jan Ingo Flege[2,3], and Markus Donath[1] — [1]University of Münster, Germany — [2]Brandenburg University of Technology Cottbus-Senftenberg, Germany — [3]University of Bremen, Germany

Spin-polarization detectors are employed in photoemission experiments to reveal the spin texture of electronic states. One well-proven approach is based on the VLEED process, where the spin-dependent electron reflection from targets influenced by exchange and/or spin-orbit interaction is used. The suitability of a target must be investigated beforehand [1,2]. In this talk, a first impression of TMDC-based detectors is given [3]. The spin-dependent electron reflectivity of spin-orbit-influenced MoS_2 is measured over a wide range of incident energies and angles for the following samples: a single layer of MoS_2 on Au(111) and cleaved MoS_2 single-crystal surfaces. On the basis of the resulting maps for the electron reflectivity, Sherman function, and figure of merit, promising features of MoS_2 for use in spin-polarization detection are discussed.

[1] Thiede *et al.*, Phys. Rev. Applied **1**, 054003 (2014).

[2] Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020).
[3] Angrick *et al.*, Phys. Rev. B, accepted for publication (2025).

TT 84.7 Thu 16:30 HSZ/0204

Efficient GW calculations for metals from an accurate ab initio polarizability: the case of doped MoS2 monolayer — •Giacomo Sesti[1], Pino D'Amico[1], Alberto Guandalini[2], Claudia Cardoso[1], Andrea Ferretti[1], and Daniele Varsano[1] — [1]CNR-NANO, Modena, Italy — [2]Università di Roma La Sapienza, Roma, Italy

Many-body perturbation theory in the GW approximation has proved very successful for the calculation of quasiparticle (QP) band structures of semiconductors. QP corrections are less significant in metals and are typically disregarded for the computational cost involved. Also, GW calculations of metals suffer of specific methodological challenges to properly treat the screening. This is typically solved under the addiction of a Drude term, that however is inadequate at low dimensionalities[1]. Furtherly, even for metals, QP corrections become more relevant at lower dimensionalites.

Here, we present GW calculations of QPs for doped MoS_2 monolayer showing excellent agreement with experimental ARPES measurements[2]. Such an unprecedented agreement has been possible thanks to the W-av method, which combines a Monte Carlo integration with interpolation approaches. This technique originally developed for 2D semiconductors[3] is here extended to the metallic case.

1) Champagne et al. NanoLett. 23.10 (2023)
2) Liu et al. PRL. 122 (2019)
3) Guandalini et al., npj Computational Materials, 9 (2023)

TT 84.8 Thu 16:45 HSZ/0204

Ultrafast Momentum Dependent Relaxation Dynamics in $TbTe_3$ — •Florian Denizer[1], Noah Meyer[2,3], Anisha Singh[3], Ian R. Fisher[3], Uwe Bovensiepen[1], Zhi-Xun Shen[2,3], and Patrick S. Kirchmann[2] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Department of Physics, Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford University — [3]Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University

Rare-earth tritellurides (RTe_3) form charge density waves (CDW) due to electronic instabilities at the Fermi-surface, because of an anisotropy of the crystal lattice between the two major in-plane crystal axes a and c. Unoccupied electronic states can be populated by ultrafast laser excitation. Electronic relaxation and coherent vibrational modes including the amplitude mode have been investigated by time and angle resolved photoelectron spectroscopy (*tr*-ARPES). Among the manifold of laser-driven processes, the one that is responsible for the electronic instability has not yet been identified. With this objective in mind we perform a *tr*-ARPES experiment on $TbTe_3$ and investigate the momentum transfer along the a- and the c-axis as a function of excitation strength. At sufficiently low pump fluence below $F = 0.3$ mJ/cm^2 we identify (quasi-)elastic scattering in the vicinity of the Fermi surface. In the talk we will discuss isotropic defect-induced elastic scattering and directed quasi-elastic scattering determined by the nesting vector. Funding through the DFG within SFB 1242 and through the DOE is gratefully acknowledged.

TT 84.9 Thu 17:00 HSZ/0204

Unconventional Topological Superconductivity in CrCl3/NbSe2 heterostructures — •Souvik Das[1], Benjamin Zhou[2,3], Anshuman Padhi[1], Jing-Rong Ji[1], Niclas Heinsdorf[2,3], Prajwal Rigvedi[1], Tianzhe Chen[1], Weibin Li[4], Pierluigi Gargiani[4], Manuel Valvidares[4], Marcel Franz[2,3], Banabir Pal[1], and Stuart S.P. Parkin[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver, Canada — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada — [4]ALBA Synchrotron Light Source, Barcelona, Spain

Topological p-wave superconductors can host non-Abelian particles useful for fault-tolerant quantum computing. Here we report experimental evidence of unconventional topological superconductivity in a heterostructure of monolayer, in-plane ferromagnetic CrCl3 islands on superconducting NbSe2. STM measurements show that, despite CrCl3 being ferromagnetic, the interfacial superconducting gap is more robust against out-of-plane magnetic fields than the s-wave gap of NbSe2, indicating unconventional pairing. We also find enhanced zero-energy states along CrCl3 island edges, consistent with the presence of edge modes. Theory suggests these features arise from an intrinsic helical p-wave state stabilized by interfacial Rashba spin-orbit coupling. This demonstrates a new route to create topological superconductivity via interface engineering.

TT 84.10 Thu 17:15 HSZ/0204

Structural and Electronic Properties of CrSBr Nanoribbons: Insights from First-Principles Calculations — •Daniil Kruklinskii, Mahdi Ghorbani-Asl, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Experiments show that exfoliated CrSBr flakes naturally form nanoribbons along a specific crystallographic direction, and similar structures can be fabricated using an electron beam in the TEM as a cutting tool. Here, we employ density functional theory calculations to systematically investigate the stability as well as electronic and magnetic properties of CrSBr nanoribbons. Our results indicate that nanoribbons oriented along one of the two major crystallographic directions are the most stable under typical growth and exfoliation conditions and remain semiconducting, exhibiting pronounced electron-hole separation between the VBM and CBM. In contrast, nanoribbons in the perpendicular direction display a substantially reduced band gap due to strongly localized edge states. Both orientations retain strongly spin-polarized band-edge states near the Fermi level and show only a weak dependence of the band gap on ribbon width. Using *ab initio* molecular dynamics simulations, we further demonstrate that electron-beam irradiation with energies of at least 200 keV can facilitate the fabrication of nanoribbons directly from pristine monolayer CrSBr, favouring the formation of diagonal nanoribbons. These diagonal ribbons are metallic, in contrast to the monolayer, and host a high density of majority-spin edge states, giving rise to pseudo-half-metallic transport.

TT 84.11 Thu 17:30 HSZ/0204

Band-selective coherent phonon-driven band renormalization in 1T-$MoTe_2$ — •Carl Jensen[1], Christopher Emeis[2], Stephan Jauernik[1], Petra Hein[1], Fabio Caruso[2], and Michael Bauer[1,3] — [1]nstitute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Institute of Theoretical Physics and Astrophysics, Kiel University, 24098 Kiel, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

Understanding the coupling between coherent phonons and the electronic system is crucial for controlling nonequilibrium properties in solids. Here, we investigate mode- and band-selective electron-phonon coupling in centrosymmetric 1T-$MoTe_2$ using time- and angle-resolved photoemission spectroscopy combined with frequency-domain analysis (FDARPES). Femtosecond near-infrared pulses excite coherent Ag-symmetric phonon modes at 2.34 THz, 3.34 THz, and 3.86 THz, which manifest as oscillatory modulations in photoemission intensity and binding energy across the valence bands. Pixel-wise Fourier analysis, based on a recently developed methodology [1], reveals pronounced band selectivity with distinct coupling strengths for different electronic states and phonon modes, enabling the evaluation of band-renormalization amplitudes in the few-meV range. Ab initio calculations using DFT/DFPT qualitatively reproduce the experimentally observed coupling patterns and relative trends, demonstrating the capability of combined experimental and theoretical approaches to resolve ultrafast electron-phonon interactions in quantum materials.

[1] N. Gauthier, H. Soifer, J.A. Sobota, H. Pfau, E. J. Sie, A. M. Lindenberg, Z.-X. Shen, P. S. Kirchmann, Rev. Sci. Instrum. 96 (2025)