O 59: 2D Materials: Electronic structure, excitations, etc. II (joint session O/HL/TT)

Time: Wednesday 10:30–12:30 Location: TRE/MATH

O 59.1 Wed 10:30 TRE/MATH

Polarons in epitaxial single-layer $MnBr_2$ — •Affan Safeer, Oktay Güleryüz, Guangyao Miao, Wouter Jolie, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

We investigate polaron formation in insulating single-layer $MnBr_2$ grown by molecular beam epitaxy on three different substrates: graphene on Ir(110), graphene on Ir(111), and Au(111). The polaron number densities and species depend strongly on the underlying substrate, underscoring the crucial role of the substrate. Our findings show that modeling of polarons in such single-layer insulators in contact with conducting substrates must explicitly include the substrate. For $MnBr_2$ grown on graphene/Ir(110), we identify four distinct polaron species, three of which closely resemble those reported for $CoCl_2$ on graphite. These polarons can be created, converted, and laterally manipulated by the STM tip when a tunneling current flows at suitable bias voltages. For graphene on Ir(110) as a substrate, mobile polarons in $MnBr_2$ are guided by the periodic potential imposed by the supermoiré pattern arising from the interaction of $MnBr_2$ with graphene and Ir(110).

O 59.2 Wed 10:45 TRE/MATH

Chirality in the Kagome Metal CsV_3Sb_5 — •Tom P. Lammersköttter[1], H.J. Elmers[2], G. Schönhense[2], O. Tkach[2], Y. Lytvynenko[2], H. Agarwal[2], S. Chernov[3], M. Hoesch[3], D. Kutnyakhov[3], M. Scholz[3], K. Rossnagel[4], A. Gloskovskii[3], C. Schlueter[3], A. Winkelmann[5], A. Haghighirad[6], M. Schmitt[7], T. Lee[7], R. Claessen[8], M. Le Tacon[6], J Demsar[2], and O. Fedchenko[1] — [1]Goethe-Universität Frankfurt (Germany) — [2]JGU Mainz (Germany) — [3]DESY Hamburg (Germany) — [4]Universität zu Kiel (Germany) — [5]AGH University of Krakow (Poland) — [6]KIT Karlsruhe (Germany) — [7]DIAMOND (UK) — [8]Universität Würzburg (Germany)

Kagome metals AV_3Sb_5 (A = Cs, K, Rb) exhibit flat bands, Dirac points, and van Hove singularities that drive unconventional charge-density-wave (CDW) order and topological states. We study chirality in CsV_3Sb_5 using angle-resolved photoemission spectroscopy (ARPES) and x-ray photoelectron diffraction (XPD) with circularly polarized photons. XPD reveals a local crystal chirality in the CDW phase. ARPES shows pronounced magnetic circular dichroism (MCD), demonstrating a chiral electronic structure and indicating orbital moments possibly linked to loop-current order. To probe orbital-moment coupling, we study Nb-doped CsV_3Sb_5, where band broadening and enhanced Dirac-like gaps occur. In the CDW phase, the strongly increased MCD indicates time-reversal-symmetry breaking and couples to the three van Hove singularities at the M points.

O 59.3 Wed 11:00 TRE/MATH

Ab initio and group theory ananlysis of monolayer BiTeI — •Josep Mas-Garcia, Jorge Cervantes-Villanueva, Alejandro Molina-Sánchez, and Alberto García-Cristóbal — ICMUV - University of Valencia - Spain

Monolayer BiTeI is a prototypical polar semiconductor whose remarkable Rashba spin splitting, rooted in strong spin-orbit coupling and non-centrosymmetric structure, offers a fertile landscape for advancing two-dimensional spintronics. This work presents and ab initio and group-theoretical analysis of BiTeI. Employing fully relativistic density functional theory and GW calculations, we obtain electronic structures that serve as benchmarks for the group-theory based Hamiltonian model. Leveraging the systematic method of invariants, we construct symmetry-constrained k-p Hamiltonians near the Γ point. Our implementation of the method of invariants enables precise fitting of the Hamiltoninan eigenvalues to ab initio band dispersions for the obtention of the parameters, and yields a highly compact analytic model that reproduces Rashba splitting and symmetry-dependent features. This framework facilitates straightforward evaluation of key physical quantities, such as effective masses or spin textures, and perturbative responses including electric and magnetic fields and strain effects within a unified and transparent formalism. Moreover our methodology establishes a versatile template for the symmetry-guided modeling of nonmagnetic semiconductors with strong spin-orbit coupling.

O 59.4 Wed 11:15 TRE/MATH

Production of Interstitials in 2D Transition-Metal Dichalcogenides (TMDs) by Ion Irradiation: ab-initio Simulations — •Silvan Kretschmer[1], Joel Davidsson[2], and Kristian S. Thygesen[1] — [1]CAMD, Technical University of Denmark — [2]Department of Physics, Linköping University, Sweden

Defects critically shape the properties of two-dimensional (2D) materials and can be purposefully introduced to tune magnetic, electronic, and optical behavior. Low-energy ion irradiation has recently emerged as an effective route for generating specific defect types via direct implantation [1,2].

First-principles simulations are essential for understanding irradiation-induced defect formation [3], but DFT-based molecular dynamics (MD) is computationally costly and limits broad exploration of materials and irradiation conditions. Machine-learning (ML) interatomic potentials provide a high-accuracy, low-cost alternative, enabling efficient screening of large datasets such as the Impurities in 2D Materials Database [4].

Here, we benchmark a ML potential against ab-initio MD, emphasizing accurate treatment of the short interatomic distances occurring during ion impacts. We apply the fine-tuned ML to study interstitial defect formation in TMDs under low-energy ion irradiation, providing defect formation probabilities and identifying suitable ion-beam parameters for targeted defect engineering in 2D materials.

[1] 10.1038/s41699-022-00318-4 [2] 10.1021/acsnano.4c03475
[3] 10.1103/PhysRevMaterials.8.114003 [4] 10.11583/DTU.19692238

O 59.5 Wed 11:30 TRE/MATH

Long-living metastable electronic states in substituted $1T$-TaS_2 — •Gaël Reecht[1], Jesumony Jayabalan[1], Ričards Knipšis[2], Florian Diekmann[3], Friedemann Queisser[2], Ping Zhou[1], Walter Schnelle[4], Kai Rossnagel[3,5], Ralf Schützhold[2], Manuel Gruber[1], and Uwe Bovensiepen[1] — [1]University Duisburg-Essen, Germany — [2]HZ Dresden-Rossendorf, Germany — [3]CAU of Kiel, Germany — [4]MPI for Chemical Physics of Solids, Dresden, Germany — [5]DESY, Hamburg, Germany

$1T$-TaS_2 is a prototypical correlated material whose low-temperature phase exhibits a commensurate charge density wave forming Star-of-David (SOD) clusters. Each SOD hosts a single electron close to E_F and, due to strong on-site Coulomb repulsion, the system enters a Mott insulating state. Adding or removing an electron creates doublon or holon excitations, which typically relax within few femtoseconds [1]. Here, we manipulate the lifetime of the quasiparticle excitations by substituting some Ta with an electron richer element. Using LT-scanning tunnelling microscopy and spectroscopy (STM/STS) and time-resolved photoemission spectroscopy, we observe metastable doublons with lifetimes ranging from fs to hours. STM/STS further shows that these excitations are locally confined. The experimental observations are corroborated by a theoretical description based on a Fermi-Hubbard model. The disorder induced by the random substitution leads to a spatial localization of holon and doublon wavefunctions at the origin of the long lifetimes observed experimentally.

[1] M. Ligges et *al.*, Phys. Rev. Lett., **120**, 166401 (2018)

O 59.6 Wed 11:45 TRE/MATH

Fingerprints of Excitonic Collective Modes in the Two-Dimensional Electron Gas — •Jakob Wolff[1,2,3], Silvana Botti[2,3], Lucia Reining[4,3], and Matteo Gatti[4,3,5] — [1]Institut für Festkörpertheorie- und Optik, Friedrich-Schiller-Universität Jena, Germany — [2]Research Center Future Energy Materials and Systems, University Alliance Ruhr and Interdisciplinary Centre for Advanced Materials Simulation, Faculty of Physics and Astronomy, Ruhr University Bochum, Germany — [3]European Theoretical Spectroscopy Facility (ETSF) — [4]LSI, CNRS, CEA/DRF/IRAMIS, École polytechnique, Institut Polytechnique de Paris, France — [5]Synchrotron SOLEIL, Gif-sur-Yvette, France

We investigate the collective charge excitations of the two-dimensional homogeneous electron gas in the low density regime within the framework of time-dependent density functional theory. We show that beyond the well-known plasmons new collective excitonic modes emerge, which leave characteristic fingerprints in experimentally accessible quantities, such as asymmetric peak structures in the loss function

and enhanced Friedel oscillations. Further, at sufficiently low densities the collective modes become imaginary, indicating an instability towards the formation of a charge-density-wave phase with excitonic origin.

O 59.7 Wed 12:00 TRE/MATH

Moir'e modulated quantum spin liquid candidate 1T-TaSe2 — Ziying Wang, Adolfo O. Fumega, Ana Vera Montoto, Mohammad Amini, Büsra Gamze Arslan, Ales Cahlik, Yuxiao Ding, Jose L. Lado, •Robert Drost, and Peter Liljeroth — Aalto University, Department of Applied Physics

Quantum spin liquids continue to fascinate with their highly entangled quantum states and promises of fractional many-body excitations. Yet there are few tools to probe these materials, and none sensitive enough for applications in 2D materials. This seriously hampers the study of monolayer QSL candidates such as α-RuCl3 and 1T-TaSe2. Scanning tunneling microscopy and spectroscopy may overcome this challenge, as they can access the fundamental excitations of 2D samples through inelastic tunneling spectroscopy. These low-energy excitations can be compared against theoretical models and provide fingerprints of QSL states. We employ this approach against the quantum spin liquid candidate 1T-TaSe2. We observe the emergence of a root 3 reconstruction driven by the substrate, equivalent spectroscopy across all spin sites, and the coexistence of zero and finite energy excitations. These observations are consistent with a QSL ground state. Our results demonstrate that IETS provides a powerful route to obtain atomic-scale insight into the magnetic excitations of two-dimensional materials. Spectral fingerprints may help to identify exotic phases of matter that are otherwise difficult to detect.

O 59.8 Wed 12:15 TRE/MATH

Long-Range Interactions in Twisted Bilayer Materials with Machine Learning for the Electronic Density — •Zekun Lou[1], Alan Lewis[2], and Mariana Rossi[1] — [1]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Department of Chemistry, University of York, York, U.K.

Moiré superlattices in twisted bilayer (TB) 2D materials exhibit extraordinary quantum phenomena, but first-principles understanding remains limited by computational costs. While most machine learning (ML) methods for density functional theory (DFT) acceleration are based on the locality assumption, we demonstrate that accurate moiré electronic structure prediction requires long-range encoding due to charge rearrangement, orbital hybridisation, and moiré potential modulation. Using long-range representations [1] for electronic-density prediction [2,3], we achieve low-energy band-structure predictions with $<$15 meV errors across twisted bilayer graphene (TBG), hBN, and transition-metal dichalcogenides (TMDCs), while $\sim$100 times faster than DFT. Descriptor requirements are material-dependent: homoatomic systems (e.g., TBG) are well-described by local descriptors, while hBN and TMDCs require long-range encoding. We summarise the physical implications of these findings that marry machine learning and the fundamental physics that governs the electronic density of twisted bilayer materials.

[1] A. Grisafi, M. Ceriotti, JCP 151, 204105 (2019)
[2] A. Lewis, A. Grisafi, M. Ceriotti, M. Rossi, JCTC 17, 7203 (2021)
[3] A. Grisafi, A. Lewis, M. Rossi, M. Ceriotti, JCTC 19, 4451 (2023)