# O 61: 2D Materials: Electronic Structure and Exitations II (joint session O/HL/TT)

Time: Wednesday 10:30–12:45 Location: H11

O 61.1 Wed 10:30 H11

**The Bell-Shaped Component in Diffraction from 2D Materials** — •Birk Finke[1], Christian Brand[1], Karim Omambac[1,2], Pascal Dreher[1], Hannah Kohler[1], Frank-J. Meyer zu Heringdorf[1,3,4], and Michael Horn-von Hoegen[1,3] — [1]Universität Duisburg-Essen — [2]Polytechnique Montréal Canada — [3]Center for Nanointegration Duisburg-Essen — [4]Interdisciplinary Center for Analytics on the Nanoscale

In 2D materials, the formation of moiré superlattices with graphene or hBN on crystalline surfaces alters electronic, vibrational, and chemical properties. Here we analysed an unusual broad diffraction background observed in low energy electron diffraction from 2D material systems, which is called the bell-shaped component (BSC). Employing SPA-LEED, LEEM, and $\mu$-LEED we propose the origin to be the inelastic scattering of the low energy electrons at the vertically polarized ZA-phonons of the weakly bound graphene and hBN layers on Ir(111) and SiC(0001). For these systems the ZA-phonon branch exhibits a parabolic dispersion with a finite phonon frequency of a few meV at the $\Gamma$ point. This results in a high phonon density at low energy, but high momentum causing the strong intensity of the BSC in diffraction. In the framework of kinematic scattering theory, we performed simulations of the inelastic diffuse scattering which quantitively confirm our proposal.

O 61.2 Wed 10:45 H11

**Combining DFT and ML to Explore the Electronic Properties of Nano-porous Graphene** — •Bernhard Kretz and Ivor Lončarić — Institut Ruder Bošković, Zagreb, Croatia

Nano-porous graphene (NPG) holds great potential in electronics due to its tunable electronic properties. However, establishing a comprehensive understanding of how structural parameters influence these properties remains a challenge. This work employs density functional theory (DFT) calculations combined with machine learning (ML) to systematically investigate both static and dynamic electronic properties across a set of 460 NPG structures derived from four distinct templates.

Our DFT results reveal correlations between structural features and band gaps within subsets of our NPG structures. Notably, we identify certain NPG configurations exhibiting band gap behavior analogous to armchair graphene nano-ribbons. To predict the dynamic response of our NPG structures, we train two distinct ML networks: one for predicting forces and total energies, and another one for predicting band gaps. Using the former allows us to perform temperature-dependent molecular dynamics simulations for all 460 NPG structures, while the latter enables us to predict band gap evolution under varying operating temperatures, a crucial factor for semiconductor device performance. Our findings identify several NPG structures exhibiting band gaps suitable for semiconductor applications while demonstrating sufficient thermal stability to function effectively at typical operating temperatures.

**Invited Talk** O 61.3 Wed 11:00 H11

**Polaritons in two-dimensional materials and hybrids probed by electron beams** — •Nahid Talebi — Institute for Experimental and Applied Physics, Kiel University, Leibnizstr. 19, 24118 Kiel

Polaritonic quasiparticles in two-dimensional (2D) materials have garnered significant attention in recent years, emerging as a promising platform for studying novel photon- and phonon-mediated correlations between various material excitations. In this work, we employ electron beams to investigate exciton and plasmon polaritons in diverse 2D materials, including transition-metal dichalcogenides, perovskites, hexagonal boron nitride, borophene, and hybrid systems. By comparing cathodoluminescence and photoluminescence spectroscopy, we uncover differences in the selection rules governing the excitation of quasiparticles by coherent light versus electron beams. Furthermore, leveraging a recently developed method that utilizes electron-driven photon sources inside an electron microscope for Ramsey-type spectroscopy, we examine the coherence of cathodoluminescence emitted by exciton polaritons (Nature Physics 19, 869 (2023)) and defects in hexagonal boron nitride (arXiv:2404.09879). These results provide new insights into the temporal coherence of the radiation from 2D materials excited by coherent and incoherent excitations.

O 61.4 Wed 11:30 H11

**Electron-phonon interaction in polar two-dimensional materials** — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial effect in solid state physics, in particular in two-dimensional materials. We recently developed a generally applicable ab-initio implementation on top of density functional theory that combines finite differences calculations with the perturbative Allen-Heine-Cardona framework in order to calculate the temperature-dependent renormalization of the electronic bandstructure due to electron-phonon interaction using a basis set of localized Gaussian orbitals. Our implementation circumvents the limiting problems of previous implementations and allows to evaluate Debye-Waller contributions beyond the rigid-ion approximation, which are usually neglected [1].

Incorporating effects from macroscopic electric fields into our implementation allows us to extend our calculations to the class of polar materials. In this presentation we discuss our results for two-dimensional transition-metal dichalcogenides, where the renormalization of the electronic bandstructure due to electron-phonon interaction can be as large as several hundreds of meV.

[1] Mann et al., Phys. Rev. B **110**, 075145 (2024)

O 61.5 Wed 11:45 H11

**Structural modulations of unidirectional charge density waves in rare earth tellurides** — •Eunseo Kim[1], Sanghun Lee[1], Junho Bang[1], Hyungryul Yang[1], Jongho Park[2], Changyoung Kim[2], Dirk Wulferding[2], Doohee Cho[1], Makoto Hashimito[3], Donghui Lu[3], and Sunghun Kim[4] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Republic of Korea — [3]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — [4]Department of Physics, Ajou University, Suwon 16499, Korea

Charge density waves (CDWs) in rare earth tellurides ($RTe_3$) provide a unique platform for exploring the interplay between lattice deformations and electronic order. Using scanning tunneling microscopy and spectroscopy (STM/S), we investigate unique surface features in two different materials, $GdTe_3$ and $DyTe_3$, that influence the CDW behavior. In $GdTe_3$, twin domain boundaries provide a static platform for observing the spatial "melting" of unidirectional CDWs and the emergence of bidirectional CDWs. Our spatial lock-in analysis demonstrates the attenuation of CDW order parameters and the proliferation of topological defects at these boundaries, correlating with enhanced local density of states near the Fermi level. In $DyTe_3$, nanowrinkles act as topological interfaces, hosting phase-winding CDWs and confining one-dimensional metallic states. These findings emphasize the role of local structural distortions in shaping CDW phenomena, offering insights into manipulating quantum states via lattice engineering.

O 61.6 Wed 12:00 H11

**Ultrafast Charge Separation on the Nanoscale Induced by a Uniform Field** — •Jan-Philip Joost and Michael Bonitz — Kiel University, Institute for Theoretical Physics and Astrophysics, 24098 Kiel, Germany

When illuminated by white light, atoms, molecules, and materials absorb only certain characteristic energy contributions based on their absorption properties. Here, we show that this effect can be translated from energy to space: a spatially uniform laser pulse can create strongly localized carrier excitations and spatial charge separation on the sub-nanometer scale within a few femtoseconds, possibly opening new avenues for nanoelectronics. A promising candidate are small graphene heterostructures, which exhibit a pronounced space dependence of the DOS with strongly localized topologically protected states [1]. Direct evidence for this effect is presented by performing extensive NEGF simulations for these systems that take into account strong coupling and dynamical screening [2]. Further, we demonstrate multiple ways to excite targeted areas of the nanostructures, such as a proper choice of the laser energy, polarization, or carrier-envelope phase. Moreover, we find that the observed effects greatly benefit from surface screening, while in free-standing systems the targeted charge

excitation is restricted by strongly bound excitons. The findings are expected to be applicable for a broad class of nanoscale monolayer clusters of graphene or TMDCs.

[1] J.-P. Joost et al., Nano Lett. **19**, 9045 (2019)
[2] J.-P. Joost et al., Phys. Rev. B **105**, 165155 (2022)

O 61.7 Wed 12:15 H11

**Two-dimensional breathing Kagome lattice of antimony atoms on a SiC substrate** — •Bing Liu[1], Kyungchan Lee[1], Jonas Erhardt[1], Manish Verma[1], Stefan Enyner[1], Cedric Schmitt[1], Philipp Kessler[1], Lukas Gehrig[1], Chris Jozwiak[2], Aaron Bostwick[2], Martin Kamp[1], Eli Rotenberg[2], Jörg Schäfer[1], Simon Moser[1], Giorgio Sangiovanni[1], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

The Kagome lattice, characterized by flat electronic bands, which represents a class of candidate materials for charge order, time-reversal symmetry-breaking and exotic superconductivity. In this work, we report the successful synthesis of a breathing Kagome lattice of Sb on SiC surface. Band mapping reveals a significant gap opening at the K point near the Fermi level, driven by different hopping parameters within the breathing Kagome lattice. Scanning tunneling microscopy measurements of this phase confirm a well-ordered 2x2 lattice reconstruction, consistent with the breathing Kagome unit cell. Furthermore, DFT calculations elucidate the role of the Sb p-orbitals. Specifically, near the Fermi level the physics is dominated by px and py orbitals, which are sensitive to hopping and possibly electron correlation, giving rise to an energy gap, and by their splitting reflect the breathing Kagome lattice situation. Our findings demonstrate a pathway for constructing two-dimensional Kagome lattices on semiconductor surfaces, and are encouraging further research into their spin and electronic properties.

O 61.8 Wed 12:30 H11

**Ultrafast lattice dynamics of monolayer $ReS_2$** — •Victoria C. A. Taylor[1], Yoav W. Windsor[1,2], Samuel Lai[3], Hyein Jung[1,2], Fang Lui[3], and Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Technische Universität Berlin, 10623 Berlin, Germany — [3]Stanford University, Stanford, CA 94305, USA

Within the transition metal dichalcogenide (TMDC) material family, TMDCs containing rhenium stand out due to their low crystal symmetry. Instead of the common hexagonal structure, $ReS_2$ exhibits in-plane 1D chains of rhenium ions due to a Peierls-like distortion. This highly anisotropic crystal structure results in a range of material properties, such as anisotropic effective carrier masses, polarization dependent optical absorption, and extremely weak interlayer coupling.

We present femtosecond electron diffraction (FED) measurements of monolayer $ReS_2$. FED is a direct probe of photoexcited lattice dynamics, providing quantitative information on coherent and incoherent atomic vibrations on femtosecond timescales. In $ReS_2$ monolayers we observe a strong and complex lattice response to photoexcitation. In particular, we observe a rapid ($<$1 ps) collective response, indicative of a concerted change in ionic positions within the unit cell. We measure the fluence dependence of this response and investigate the effect of the pronounced polarization dependence of the optical excitation, which results from the material's in-plane anisotropy.