O 44: 2D Materials III: Electronic Structure (joint session O/TT)

Time: Wednesday 10:30–13:00 Location: MA 005

O 44.1 Wed 10:30 MA 005

Semiclassical theory for plasmons in inhomogeneous two-dimensional systems — •Tjacco Koskamp, Koen Reijnders, and Mikhail Katsnelson — Radboud University, Nijmegen, The Netherlands

We construct a general theory for plasmons in inhomogeneous two-dimensional systems. Plasmons, quantized collective oscillations of conduction electrons in solids, can be used to manipulate and control light. This requires heterostructures of nanometer size, which are by definition spatially inhomogeneous, and difficult to describe analytically. Here, we present a novel semi-analytical method to describe plasmons in two-dimensional inhomogeneous media within the framework of the Random Phase Approximation (RPA). Our approach [1] is based on the semiclassical approximation, which is formally applicable when the length scale of the inhomogeneity is much larger than the plasmon wavelength. Within this framework, we obtain a classical Hamiltonian that describes the dynamics of quantum plasmons, given by the Lindhard function with spatially varying parameters. The classical trajectories generated by this Hamiltonian can be viewed as the analog of rays in geometrical optics. By subsequently adding the wave-like character of the plasmons to these classical trajectories, we can describe, for instance, plasmon scattering and plasmonic bound states. As an example, we compute the differential cross section for plasmon scattering by a radially symmetric impurity.

[1] T. M. Koskamp, M. I. Katsnelson, K. J. A. Reijnders, Phys. Rev. B 108, 085414 (2023)

O 44.2 Wed 10:45 MA 005

Imaging dielectric near-field modes of hexagonal boron nitride by photoemission electron microscopy — •Yaolong Li[1,2], Martin Aeschlimann[2], Quan Sun[1], Yunan Gao[1], Xiaoyong Hu[1], and Qihuang Gong[1] — [1]Department of Physics, Peking University, Beijing, China — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern-Landau, Germany

Low-loss dielectric modes are important features and functional bases of fundamental optical components in on-chip optical devices. However, dielectric near-field modes are challenging to reveal with high spatiotemporal resolution and fast direct imaging. Here, we present a method to address this issue by applying time-resolved photoemission electron microscopy to a low-dimensional wide-bandgap semiconductor, hexagonal boron nitride (hBN). Using a low-loss dielectric planar waveguide as the fundamental structure, static vector near-field vortices with different topological charges and the spatiotemporal evolution of waveguide modes are directly revealed. With the lowest order vortex structure, strong nanofocusing in real space is realized. Near-vertical photoemission in momentum space and narrow spread in energy space are simultaneously observed due to the atomically flat surface of hBN and the small photoemission horizon set by the limited photon energies. Our approach provides a strategy for the realization of flat photoemission emitters. Revealing low-loss dielectric near-field modes of hexagonal boron nitride by photoemission electron microscopy. Nat. Commun. 14, 4837 (2023).

O 44.3 Wed 11:00 MA 005

Noble metal dichalcogenides: Optoelectronic and non-linear response — George de Coster[1], Stefan Heiserer[1], Simon Schlosser[1], Zdenek Sofer[2], Tanja Stimpel-Lindner[1], Georg Duesberg[1], and •Paul Seifert[1] — [1]Institute of Physics, University of the Bundeswehr Munich, Faculty of Electrical Engineering and Information Technology, Werner-Heisenberg-Weg. 39, 85577 Neubiberg, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic

Noble metal dichalcogenides belong to the material class of layered 2D materials. In particular, these materials transition from direct band gap semiconductor to semi-metal with increasing layer thickness and were shown to host type-II Dirac semi-metallic behavior, as well as topological surface states and superconductivity [1,2]. We analyze the low-frequency optoelectronic response of PdTe2 using THz time domain spectroscopy. Frequency resolved measurements reveal signatures of second order non-linear response whose symmetry constrains are consistent with the occurrence of anisotropy in its optoelectronic response to THz radiation [3]. The latter is verified in polarization resolved THz spectroscopy. The optical response at higher energies likewise exhibits this anisotropy. Our results elucidate the spectral optoelectronic response in PdTe2 at low energies and discuss its anisotropy in light of its underlying symmetry constraints. References: [1] W. Zheng et al., PRB 97, 235154 (2018) [2] O.J. Clark et al., PRL 120, 156401 (2018) [3] C. Guo et al. Sci. Adv. 6, 36 (2020)

O 44.4 Wed 11:15 MA 005

On the the nature of transient and metastable nonequilibrium phases in 1T-TaS2 — •Tanusree Saha[1,2], Arindam Pramanik[3], Barbara Ressel[1], Alessandra Ciavardini[1], Primož Rebernik Ribič[4], and Giovanni De Ninno[1,4] — [1]University of Nova Gorica, 5270 Ajdovščina, Slovenia — [2]Universität Duisburg-Essen, 47057 Duisburg, Germany — [3]Tata Institute of Fundamental Research, Mumbai 400005, India — [4]Elettra Sincrotrone Trieste, 34149 Trieste, Italy

Photoexcitation of materials with complex ground states can drive them into new out-of-equilibrium phases. In this talk, I will present the characteristics of these phases and the recovery dynamics in a complex system, the charge density wave (CDW)-Mott insulator 1T-TaS2, studied using time- and angle-resolved photoemission spectroscopy. We observe strong similarities between the band structures of the transient phase and the structurally undistorted equilibrium phase, with evidence for the coexistence of insulating and metallic phases. Following the transient phase, we find that the restorations of Mott and CDW orders begin around the same time, highlighting that the Mott transition is tied to the CDW distortion. During recovery, a metastable phase, driven by the CDW lattice order, emerges but only in the strong photoexcitation regime and is a commensurate CDW-Mott insulating phase but with a smaller CDW amplitude. Finally, I will briefly discuss our future work, where we aim to study how the nature of the metastable phase and electron correlations in photoexcited 1T-TaS2 can be tuned by an external parameter, e.g. pump fluence.

O 44.5 Wed 11:30 MA 005

Self-hybridized exciton-polaritons in thin films of Ruddlesden-Popper-Perovskites — •Maximilian Black[1], Parsa Darman[2], Sara Darbari[2], and Nahid Talebi[1] — [1]Institute for Experimental and Applied Physics, Kiel University, 24118 Kiel, Germany — [2]Faculty of Electrical and Computer Engineering, Tarbiat Modares University, 14115-111 Tehran, Iran

Lead halide perovskites have emerged as platforms for exciton-polaritonic studies at room temperature thanks to their excellent photoluminescence efficiency and great synthetic versatility. In this work we find proof of strong exciton-photon coupling in cavities formed by the layered crystals themselves, a phenomenon known as self-hybridization effect. We use multi-layers of high quality Ruddlesden-Popper perovskites in their 2D crystalline form, benefiting from their quantum-well excitonic resonances and the strong Fabry-Perot resonances resulting from the total-internal-reflection at their smooth surfaces. Optical spectroscopy reveals bending of the cavity modes typical for exciton-polariton formation, and photoluminescence spectroscopy shows thickness dependent splitting of the excitonic resonance. Additionally, local optical excitation of the flakes in photoluminescence measurements unveils long in-plane propagation of the excited modes. In previous works the influence of the incident angle is often overlooked, motivating this work to focus on tuning the in-plane momentum of the incident light to the polaritonic resonances. We therefore pave the way towards an effective way to study the rich physics of exciton-polaritons in Ruddlesden-Popper 2D perovskites.

O 44.6 Wed 11:45 MA 005

Inelastic tunneling into polaronic bound states in single-layer MoS_2 — Camiel van Efferen[1], Arne Schobert[2], Tfyeche Tounsi[1], Michael Winter[2], Mark Georger[1], Affan Safeer[1], Christian Krämer[1], Jeison Fischer[1], Jan Berges[3], Thomas Michely[1], •Roberto Mozara[2], Tim Wehling[2,4], and Wouter Jolie[1] — [1]II. Physikalisches Institut, U zu Köln — [2]I. Institut für Theoretische Physik, U Hamburg — [3]U Bremen Excellence Chair, Bremen Center for Computational Materials Science, and MAPEX Center for Materials and Processes — [4]The Hamburg Centre for Ultrafast Imaging

The presentation delves into the nuanced conductivity of two-dimensional MoS_2, a prominent transition metal dichalgogenide, by examining its response to doping-induced variations. In particular, we explore the intriguing phenomena of polarons, quasiparticles that emerge from the interplay of electrons with lattice vibrations. Employing advanced techniques such as scanning tunneling microscopy and spectroscopy, we unveil the manifestation of polaronic bound states in metallic 2D MoS_2, shedding light on their stability and formation dynamics. The investigation is enriched by density-functional theory calculations with a recently developed electron-lattice downfolding technique, emphasizing the role of renormalized M-phonons in shaping the electronic landscape of metallic MoS_2. This synthesis of experimental insights and theoretical perspectives offers a comprehensive understanding of the interplay between electrons and phonons in 2D MoS_2.

O 44.7 Wed 12:00 MA 005

Strain-dependent electromechanical and optoelectronic properties of free-standing PtSe2 films — •Natalie Galfe, Stefan Heiserer, Maximilian Wagner, Michael Loibl, Silke Boche, Simon Schlosser, Oliver Hartwig, Tanja Stimpel-Lindner, Cormac Ó Coileáin, Kangho Lee, George de Coster, Paul Seifert, and Georg S. Duesberg — University of the Bundeswehr Munich

We report on the piezoresistive and optoelectronic properties of free-standing noble metal dichalcogenide $PtSe_2$ films under controlled strain. Bridges of polycrystalline $PtSe_2$ films with different geometries were fabricated directly on target substrates. The pre-structered platinum channels were selenized through thermally assisted conversion and the resulting $PtSe_2$ electrically contacted and underetched. The controlled strain of the bridges was induced by application of back-gate voltages. This makes them an excellent platform to study the impact of strain on transport and optoelectronic properties.

Increasing tensile strain shows a decrease in the electrical resistance, which is attributable to an enhancement of the density of states at the Fermi level. Raman analysis of the channel under increasing static strain displays a blue-shift of the Raman modes, which can be attributed to a decrease in effective film thickness which is supported by finite element simulations of the polycrystalline films. By applying AC gate voltages, the geometry-dependent eigenfrequencies of the bridges can be determined proving their expected mechanical oscillations. The results lead to a deeper understanding of this novel material class and serve as a platform for further applications.

O 44.8 Wed 12:15 MA 005

Direct visualization of conduction band electrons in gated single layer TMDC via micro ARPES — •Chakradhar Sahoo[1], Yann in 't Veld[2], Alfred J. H. Jones[1], Zhihao Jiang[1], Paulina E. Majchrzak[1], Kimberly Hsieh[1], Kenji Watanabe[3], Takashi Taniguchi[4], Yong P. Chen[1], Jill A. Miwa[1], Malte Rösner[2], and Søren Ulstrup[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark — [2]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, the Netherlands — [3]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba 305-0044, Japan — [4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba 305-0044, Japan

Electric field induced doping effects in the electronic structure of single-layer (SL) semiconductors is crucial for electronic and optoelectronic applications. However, direct visualization of doped electronic structure remains challenging for in situ gated devices. Here, we apply in operando micrometer scale angle-resolved photoemission spectroscopy at the ASTRID2 light source to characterize the electronic structure of a SL WS2 gated device. Using micromechanical cleaving and transfer methods, the SL WS2 is partially contacted to a graphene top electrode and placed on a boron nitrite dielectric on a graphite back-gate. We directly visualize distinct conduction band populations, band gap renormalization and charge transfer processes across the bare WS2 and graphene/WS2 interface. Our observations provide a better understanding of band renormalization and carrier doping in 2D devices.

O 44.9 Wed 12:30 MA 005

Deexcitation of highly charged ions at surfaces — •Anna Niggas, Matthias Werl, Daniel Thima, Filip Vukovic, Matthias Bernhart, Friedrich Aumayr, and Richard A. Wilhelm — TU Wien, Institute of Applied Physics, Vienna, Austria

Strong electronic excitations at the nanoscale can trigger nanopore formation on 2D materials and their heterostructures. One possible way to achieve these excitations are impacts of slow highly charged ions (HCIs), e.g., Xe^{40+} ions: Upon approaching the surface, resonant electron transfer leads to a population of high-n shells of the ion, with subsequent radiative and non-radiative decay, resulting in energy deposition in the very first surface layers of the material.

To unravel these deexcitation dynamics, we employ a complex coincidence spectrometer to detect correlated pairs of HCIs transmitted through 2D materials and electrons emitted from the material due to the ion impact. Filtering options for ion charge state, scattering angle, and energy loss, as well as electron number and energy, can be used for a detailed analysis of deexcitation channels. For instance, a charge-state-separated analysis of the HCI-induced electron yield from graphene shows that the number of emitted electrons increases continuously with the number of electrons captured by the projectile, reaching up to $100\,e^-$ per incident ion. Furthermore, we observe a sudden increase in the electron yield for ions filling up their valence shell.

In this contribution, we will discuss how these coincidence measurements help us understand the deexcitation of HCIs and how we can use our method to access material properties.

O 44.10 Wed 12:45 MA 005

Ultrafast Electron Diffuse Scattering as a Tool for Studying Phonon Transport: Phonon Hydrodynamics and Second Sound Oscillations — •Laurenz Kremeyer[1], Tristan Britt[1], Bradley Siwick[1,2], and Samuel Huberman[3] — [1]Department for Physics, McGill University, Montreal, Canada — [2]Department for Chemistry, McGill University, Montreal, Canada — [3]Department of Chemical Engineering, McGill University, Montreal, Canada

Hydrodynamic phonon transport phenomena, like second sound, have been observed in liquid Helium more than 50 years ago. More recently second sound has been observed in graphite at over 200 K using transient thermal grating techniques[1]. In this work we explore the signatures of second sound in ultrafast electron diffuse scattering (UEDS) patterns. We use density functional theory and solve the Boltzmann transport equation to determine time-resolved non-equilibrium phonon populations and subsequently calculate one-phonon structure factors and diffuse scattering patterns to simulate experimental data covering the regimes of ballistic, diffusive, and hydrodynamic phonon transport. For systems like graphite, UEDS is capable of extracting time-dependent phonon occupancies across the entire Brillouin zone [2] and ultimately lead to a more fundamental understanding of the hydrodynamic phonon transport regime.

[1] Ding et al. *Nat. Comm.* **13** 285 (2022)
[2] René de Cotret et al. *Phys. Rev. B.* **100** 214115 (2019)