HL 25: Poster 2D Materials: Electronic Structure and Exitations (joint session O/HL)

Time: Tuesday 13:30–15:30 Location: P3

HL 25.1 Tue 13:30 P3

Spin-orbit coupling in non-van der Waals 2D materials — •Mani Lokamani[1], Gustav Bihlmayer[2], Gregor Michalicek[2], Daniel Wortmann[2], Stefan Blügel[2], and Rico Friedrich[1,3,4] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]Forschungszentrum Jülich — [3]TU Dresden — [4]Duke University, Durham, USA

In recent years, the emerging class of non-van der Waals 2D materials has attracted considerable interest due to the unique electronic and magnetic properties of the representatives [1]. We study here the role of spin-orbit coupling (SOC) in these non-van der Waals 2D systems and related effects that might eventually lead to topological properties. With several 2D candidates including heavy elements such as Bi and Tl, significant effects due to SOC are present in the electronic structure. For the initial screening, we employ AFLOW [2] with its standardized workflows. In a second step, we retrieve the metadata using AFLOW and adapt the extracted parameters with an AiiDA-plugin [3] for accurate electronic structure calculations using the full-potential all-electron program FLEUR [4] within AiiDA. We discuss the effect of SOC on the band structures and densities of states and also focus on the topologically protected 1D conduction edge channels [5].

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[2] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).
[3] G. Pizzi *et al.*, Comput. Mater. Sci. **111**, 218 (2016).
[4] The FLEUR project: https://www.flapw.de.
[5] M. Lokamani *et al.*, manuscript in preparation (2024).

HL 25.2 Tue 13:30 P3

Influence of surface relaxations on scanning probe microscopy images of the charge density wave material $NbSe_2$ — Nikhil S. Sivakumar[1], Joost Aretz[1], •Sebastian Scherb[1], Marion van Midden Mavric[2], Nora Huijgen[1], Umut Kamber[3], Daniel Wegner[1], Alexander A. Khajetoorians[1], Malte Rösner[1], and Nadine Hauptmann[1] — [1]IMM, Radboud University, Nijmegen, The Netherlands — [2]Jožef Stefan Institute, Ljubljana, Slovenia — [3]Joseph Henry Laboratories and Department of Physics, Princeton University, Princeton, USA

Scanning tunneling microscopy (STM) images of the charge density wave (CDW) in 2H-$NbSe_2$ at voltages around the Fermi level lack a contrast inversion expected for a single-band CDW. Recent works have ascribed this to a multiband CDW or the displacement of the surface Se atoms. While STM cannot disentangle geometric and electronic structure variations, non-contact atomic force microscopy (nc-AFM) can provide better characterization of the geometric structure due to its sensitivity to the interaction between the charge densities of tip and surface. We employ distance-dependent combined constant-height STM/nc-AFM measurements to characterize the surface relaxations of 2H-$NbSe_2$. Nc-AFM images show different image contrasts depending on distance. Based on ab-initio calculations, we show that the contrast at small distances is dominated by the displacement of the surface Se atoms. For large distances, the contrast is dominated by the interaction of the permanent dipole of the tip with the potential above the surface that is predominantly modulated by the underlying Nb atoms.

HL 25.3 Tue 13:30 P3

Investigation of the electronic structure of 1T-$Ta_{1-x}Mo_xS_2$ using 11eV-laser ARPES — •Adina Timm[1,2], Florian K. Diekmann[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

The ability to modify the electronic structure of quantum materials by controlling charge density waves (CDWs) offers various possibilities for use in next-generation technologies as electronic and optoelectronic components. A material platform for testing this approach is 1T-TaS_2, which exhibits different temperature-dependent CDWs that we aim to tune by doping. Using 11eV-laser ARPES, we determine the differences in the electronic band structure of both doped and pristine TaS_2 crystals. The dopant molybdenum was introduced into TaS_2 during crystal growth by chemical vapor transport. The photoemission results show that different CDW phases are present at low doping concentrations of less than one percent with modified transition temperatures.

HL 25.4 Tue 13:30 P3

Magnetic properties of V-doped WSe2 — •Jules M. Knebusch[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Florian K. Diekmann[1,2], Adina Timm[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics holds promise for highly efficient classical and quantum computing and is therefore considered a key technology for future innovation. Pristine tungsten diselenide (WSe_2), known as a semiconductor with a two-dimensional hexagonal 2H structure, is expected to transform into a room-temperature dilute ferromagnetic semiconductor upon vanadium doping, making it a highly attractive candidate for spintronic applications. This assumption is supported by density functional theory calculations and scanning transmission electron microscopy studies, and RKKY interactions are predicted as the driving mechanism. The crystals investigated in this study were synthesized in-house employing the chemical vapor transport method. This process produced as-is vanadium-doped WSe_2 crystals with approximately 2% of the tungsten atoms (presumably) substituted by vanadium. The results reported here were obtained using a Physical Property Measurement System (PPMS) in ACMS configuration and provide valuable insights into the magnetic characteristics of this doped material.

HL 25.5 Tue 13:30 P3

Polarons in single-layer MoS_2 via downfolding approach to the coupling of electronic and nuclear degrees of freedom — •Laura Pätzold[1], Camiel van Efferen[2], Arne Schobert[1], Tfyeche Y. Tounsi[2], Michael Winter[1], Mark Georger[2], Afan Safeer[2], Christian Krämer[2], Jeison Fischer[2], Jan Berges[3], Thomas Michely[2], Roberto Mozara[1], Wouter Jolie[2], and Tim O. Wehling[1,4] — [1]U Hamburg — [2]U Köln — [3]U Bremen — [4]The Hamburg Centre for Ultrafast Imaging

A polaron is a quasiparticle describing a localized bound state resulting from the interaction of charge carriers with lattice vibrations. Though they are a well-studied phenomenon, experimental observations of polarons in 2D crystals are sparse. Here, we present the theoretical analysis of polaronic distortions in n-doped single-layer MoS_2 via a downfolding approach with linear electron-lattice coupling based on density functional theory calculations [1]. With this, a multi-polaronic distortion, caused by a renormalized M-point phonon, can be stabilized on supercells of up to 18×18. We compare our results to scanning tunneling microscopy measuremens obtained on n-doped single-layer MoS_2, which support the existence of polarons emerging from the coupling of non-polar zone-boundary phonons to Bloch electrons. This tunneling into the vibrationally coupled polaronic states is visible through evenly spaced peaks around the Fermi energy in the differential conductance, whose spacing matches the frequency of the M-point phonon responsible for the multi-polaronic distortion in our simulations.

[1] A. Schobert et al., *SciPost Phys.* **16**, 046 (2024)

HL 25.6 Tue 13:30 P3

Electronic and phononic characterization of 2H-NbS2 at the atomic scale — •Werner M.J. van Weerdenburg, Margarete Huisinga, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMDs) are a class of layered materials that can exhibit a variety of electronic properties, including low-temperature quantum phases such as superconductivity and charge density wave (CDW) formation. These phases may coexist, for instance in 2H-NbSe2, and electron-phonon interactions have been suggested as a common driving factor for the two phases [1]. In contrast, the similar compound 2H-NbS2 has a comparable superconducting critical temperature, but lacks a CDW phase [2], highlighting the importance of subtle differences in electron-phonon interactions.

Here, we apply scanning tunneling microscopy and spectroscopy (STM/STS) to investigate the electronic and phononic properties of 2H-NbS2 at the atomic scale. Based on quasiparticle interference mapping, we probe the spatial variation of the electronic density of states and identify the dispersion of the band structure around the Fermi level. Moreover, inelastic excitation spectroscopy reveals the phononic excitations of the material. By mapping the atomic-scale variation of phononic excitations around intrinsic defects of the material and adatoms, we study how electrons and phonons interact at the atomic scale.

[1] Rossnagel et al., PRB 64, 235119 (2001)
[2] Heil et al., PRL 119, 087003 (2017)

HL 25.7 Tue 13:30 P3

Characterization of surficial defect states in Mott insulator 1T-TaS_2 — •Junyoung Sim, Vibhuti Rai, Christian Lotze, and Katharina J. Franke — Freie Universtät Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

The Mott insulating state in 1T-TaS_2, arising from strong correlations among unpaired electrons within its charge density wave superlattice, is distinct from a trivial band insulator and serves as a model system for exploring the dynamics of exotic many-body states [1]. Here, we investigate bulk 1T-TaS_2 using scanning tunneling microscopy (STM) at 5 K. We find arious nanoscopic defects including vacancies, and domain. Additionally, we adsorb transition metal adatoms on the bare surface. Using tunneling spectroscopy, we map out their electronic signatures and compare them to prior studies [2].

[1] Hellmann et al. Phys. Rev. Lett. 105, 187401 (2010)
[2] Fei et al. AAPPS Bull. 32, 20 (2022)

HL 25.8 Tue 13:30 P3

FinEstBeAMS: a multipurpose VUV and soft X-ray beamline at the max iv laboratory — •Weimin Wang, Antti Kivimäki, Kirill Chernenko, Calle Preger, and Stephan Appelfeller — MAX IV Laboratory, Lund University, PO Box 118, SE-22100 Lund, Sweden

The Finnish-Estonian Beamline for Atmospheric and Materials Science (FinEstBeAMS), located at the 1.5 GeV storage ring of the MAX IV Laboratory (Lund, Sweden), is a multidisciplinary beamline that was designed to fulfil the various needs of scientific communities in atomic, molecular and optical research, surface science, and photoluminescence research.

The gas-phase end station is equipped for electron and time-of-flight ion spectroscopies in low-density matter, while the photoluminescence end station focuses on luminescence spectroscopy of solid samples. The solid-state end station is dedicated to photoelectron and X-ray absorption spectroscopy of surfaces and interfaces, utilizing a hemispherical electron energy analyzer (PHOIBOS 150 2D-DLD from SPECS). The sample is positioned via a 5-axis motorized manipulator, offering three linear and two rotational motions (polar and azimuthal). A cryostat integrated into the manipulator enables sample cooling with liquid helium (˜50 K) and nitrogen (˜90 K). Additionally, a preparation chamber allows for sample treatment and analysis using supplementary techniques.