HL 24: 2D Materials IV – Emerging materials and properties

Time: Wednesday 9:30–12:45 Location: POT/0081

HL 24.1 Wed 9:30 POT/0081

Atomic layer deposition of few-layer 1T-TiS_2 and ternary $MoTiS_2$ — •Christian Petersen[1,2], Christian Tessarek[1,2], Marco Schowalter[1,2], Andreas Rosenauer[1,2], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliothekstraße 1, 28359 Bremen, Germany

Theoretical calculations and experimental data concerning electronic and structural properties of 1T-TiS_2 are sparse in comparison to other transition metal dichalcogenides (TMD) such as MoS_2. The available data is contradicting and attributes 1T-TiS_2 a plethora of different properties ranging from a semi-metal like behaviour to different charge density wave phases (2×2 and $\sqrt{7} \times \sqrt{3}$) and even a band gap of up to 2.5 eV. In general, there is a lack of experimental data due to difficulties in synthesis and stabilization of 1T-TiS_2 which rapidly oxidizes in ambient conditions.

In this study, plasma-enhanced sub-atomic layer deposition (ALD) [1] in combination with in situ X-ray photoelectron spectroscopy (XPS) is employed to directly study the effects of the growth conditions on the chemical composition of 1T-TiS_2 while circumventing the problem of oxidation in ambient. To further characterize the 1T-TiS_2 film ex situ, Raman spectroscopy and atomic force microscopy (AFM) is utilized. Additionally, $MoTiS_2$ was synthesized by substitution of ALD cycles of the Ti precursor (TDMAT) by the Mo precursor (BTBMMo).

[1] C. Tessarek et al., 2D Mater. 11, 025031 (2024)

HL 24.2 Wed 9:45 POT/0081

The effect of Lithium intercalation on line defects in the MoS2 monolayer — •Asghar Ali Jan and Peter Kratzer — University of Duisburg-Essen, Duisburg, Germany

MoS2 can be an effective anode material in lithium-ion batteries, as it is scalable at room temperature and has weak van der Waals forces, allowing lithium ions to intercalate between the sheets. Additionally, when using MoS2 as an anode in a lithium-rich environment, the phase transition from the most stable H phase to the T' phase must also be considered. Certain defects, such as sulfur vacancies and grain boundaries, are often present in experimentally synthesized MoS2 layers. These grain boundaries introduce metallic states within the bulk band gap. As a result, the conductivity of MoS2 is reduced. Up to now, the H-to-T' phase transition in MoS2 has been extensively studied, but generally without considering the possible presence of defects such as grain boundaries. Therefore, we have investigated the interaction of lithium intercalation with the grain boundaries present in a MoS2 monolayer. For example, we examine how the presence of lithium near a mirror twin boundary (MTB) affects the one-dimensional line of charge trapped in the MTB. It is also important to consider the grain boundary formed when a T' phase created from the H phase due to lithium intercalation directly meets the remaining H phase that does not interact with lithium. Our density functional theory calculations provided insights about the stability and electronic properties of these line defects in the presence of lithiation.

HL 24.3 Wed 10:00 POT/0081

Wafer-scale growth of hexagonal boron nitride thin films using pulsed laser deposition — •Daniel Klenkert[1,2], Benedikt Winter[1], Paul Konrad[2], Andreas Sperlich[2], Vladimir Dyakonov[2], and Jens Ebbecke[1] — [1]Technology Campus Teisnach Sensor Technology, Deggendorf Institute of Technology, 94244 Teisnach — [2]Experimental Physics 6, Julius-Maximilians-University Würzburg, 97074 Würzburg

Hexagonal boron nitride (hBN) has attracted significant attention due to its wide bandgap, high thermal conductivity and its ability to host optically active defects, which are promising as single photon emitters and for quantum sensing applications. Thus far the sample preparation of hBN usually relies on tape exfoliation or high temperature chemical vapor deposition. Here we report on our progress using an alternative approach to prepare thin films of hBN on different substrates: pulsed laser deposition. This enabled the preparation of microcrystalline hBN layers on large scale wafer substrates at temperatures below 850°C. The stoichiometry preserving properties of pulsed laser deposition also allows for the preparation of carbon doped thin films. These are especially interesting for research on carbon related, optically active defects, which are noted for their high brightness and single photon purity.

HL 24.4 Wed 10:15 POT/0081

Doping-Induced Modulation of Structural and Electronic Properties in Transition Metal Dichalcogenides — •Cem Sanga[1,3], Nadire Nayir[1,3], Yusuf Kerem Bostan[2], Fahrettin Sarcan[2], Diwakar Singh[4], and Tanushree Choudhury[4] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Department of Physics, Faculty of Science, Istanbul University, Vezneciler, Istanbul, 34134, Turkey — [3]Department of Physics Engineering, Istanbul Technical University, Maslak, Istanbul, 34467, Turkey — [4]Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, Maharashtra 400076, India

Transition metal dichalcogenides (TMDCs) hold promise for electronic applications, yet their performance is limited by inadequate doping strategies. This density functional theory investigation examines substitutional and interstitial doping in MoS_2 and WS_2 using chlorine and oxygen dopants. Formation energy calculations reveal chlorine preferentially occupies sulfur vacancy sites in MoS_2. Electronic structure analysis demonstrates that strategic doping enables bandgap engineering in TMDC systems.

HL 24.5 Wed 10:30 POT/0081

Opposite In-Plane Electrical Anisotropy in $ZrSe_3$ and ZrS_3 Flakes — •Davin Höllmann[1], Lars Thole[1], Sonja Locmelis[2], and Rolf J. Haug[1,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany — [3]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, 30167 Hannover, Germany

The anisotropy in form of quasi one-dimensional (1D) chains in transition metal trichalcogenides (TMTCs) makes them stand out compared to other more conventional two-dimensional (2D) materials [1]. Through width-dependent [2] and direct measurements, we investigated the electrical properties of $ZrSe_3$ and ZrS_3 flakes, in particular, the influence of the anisotropic effective electron masses [3] in the 2D plane. Flakes with a height of 26 nm were exfoliated from the respective bulk materials grown by a chemical vapour transport method.

Despite their identical quasi 1D layered crystal structure, $ZrSe_3$ and ZrS_3 exhibit inverted in-plane electrical anisotropy. While $ZrSe_3$ exhibits the highest conductivity across the 1D chains with an anisotropy ratio of 0.60, ZrS_3 is shown to favour electron transport along the 1D chains with a ratio of 1.69. Using DFT, we attribute this to the different chalcogen contributions at the conduction band minimum.

[1] J. O. Island et al., 2D Materials 4, 0220033 (2017)
[2] D. Höllmann et al., ACS Appl. Electron. Mater. 7, 9, 4049-4054 (2025)
[3] Y. Jin et al., Phys. Chem. Chem. Phys. 17, 18665-18669 (2015)

HL 24.6 Wed 10:45 POT/0081

Observation of Bernal Stacking in Few-Layer Graphene on C face Silicon Carbide — •Jonas Rose, Oliver Brandt, Michael Hanke, Joao Marcelo Lopes, Philipp John, and Hans Tornatzky — Paul-Drude-Institut, Berlin

Epitaxial growth of few-layer graphene (FLG) on SiC($000\bar{1}$) (C face) is widely assumed to yield films with rotational disorder, in contrast to the well-ordered Bernal (AB) stacking typically associated with SiC(0001) (Si face) growth. In this work, we show that surface graphitization on the C face of SiC can, under appropriate conditions, produce FLG with genuine AB stacking and remarkably low mosaic spread. Using detailed Raman spectroscopy, supported by complementary structural characterization, we identify clear spectral signatures of Bernal ordering, including a well-defined 2D-band lineshape. These findings demonstrate that ordered stacking is achievable on the C face under controlled sublimation conditions. We will present our full spectroscopic analysis and discuss its implications for the structural and electronic properties of the grown FLG.

15 min. break

HL 24.7 Wed 11:15 POT/0081

Influence of Defects, Doping and Layer Twisting on Phonon Dispersions in Bilayer Graphene and MoS_2 from Machine-Learned Force Fields — •Sabuhi Badalov and Harald Oberhofer — Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth

In two-dimensional (2D) layered materials, phonon dispersion plays a central role in determining transport and electronic properties. In bilayer systems, phonon dispersion is highly sensitive to the stacking configuration, twist angle, defects, and doping types. Using *state-of-the-art* machine learning force fields trained on the *first-principles* data, we perform large-scale phonon calculations for bilayer graphene and MoS_2 to investigate how layer twist and defect density alter phonon spectra and interlayer vibrational modes. We also analyze the influence of p- and n-type doping on phonon dispersions and their interactions with the underlying electronic structure. Our results reveal characteristic shifts in low-energy acoustic and optical branches that are directly linked to microscopic structural motifs, including *Moiré*-induced phonon properties. These findings provide microscopic input for future calculations of electron-phonon coupling and possible phonon-mediated superconducting states in twisted and doped 2D materials and establish machine learning force fields as a powerful framework for exploring phonon-electron interaction in quantum materials.

HL 24.8 Wed 11:30 POT/0081

Efficient *GW* band structure calculations using Gaussian basis functions and application to atomically thin transition-metal dichalcogenides — •Rémi Pasquier[1], María Camarasa-Gómez[2,3], Anna-Sophia Hehn[4], Daniel Hernangómez-Pérez[5], and Jan Wilhelm[1] — [1]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, 93053 Regensburg, Germany — [2]Centro de Física de Materiales (CFM-MPC), CSIC-UPV/EHU, Paseo Manuel de Lardizabal 5, 20018 Donostia-San Sebastián, Spain — [3]Departamento de Polímeros y Materiales Avanzados: Física, Química y Tecnología, Facultad de Química, UPV/EHU, 20018 Donostia-San Sebastián, Spain — [4]Institute of Physical Chemistry, Christian-Albrechts-University Kiel, Max-Eyth-Strasse 1, 24118 Kiel, Germany — [5]CIC nanoGUNE BRTA, Tolosa Hiribidea 76, 20018 San Sebastián, Spain

The *GW* approximation is widely used to compute self-energies and related electronic properties but remains computationally demanding, motivating the development of more efficient approaches. We present a space-time *GW* algorithm for periodic systems in a Gaussian basis with spin-orbit coupling, enabling accurate and efficient quasiparticle band-structure calculations for atomically thin materials. For monolayer MoS_2, $MoSe_2$, WS_2, and WSe_2, the resulting *GW* band gaps agree on average within 50 meV with plane-wave reference values. Full G_0W_0 band structures can be computed in less than two days on a laptop (Intel i5, 192 GB RAM) or under 30 minutes using 1024 cores.

HL 24.9 Wed 11:45 POT/0081

Investigating the Ferroelectric Potential Landscape of 3R-MoS_2 through Optical Measurements — •Jan-Niklas Heidkamp[1], Johannes Schwandt-Krause[1], Swarup Deb[1,2,3], Takashi Taniguchi[4], Kenji Watanabe[4], Rico Schwartz[1], and Tobias Korn[1] — [1]Institute of Physics, University of Rostock, Rostock, Germany — [2]Homi Bhabha National Institute, Mumbai, India — [3]Saha Institute of Nuclear Physics, Kolkata, India — [4]National Institute for Material Science, Tsukuba, Japan

In recent years, sliding ferroelectricity has emerged as a topic of significant interest due to its possible application in non-volatile, reconfigurable storage devices. This phenomenon is unique to two-dimensional van der Waals materials, where out-of-plane ferroelectric polarization switching is induced by relative in-plane sliding of adjacent layers. The intrinsic stacking order influences the resulting polarization, creating distinct polarization regions separated by domain walls. These can be manipulated using an applied vertical electric field, enabling a switchable system that retains the environmental robustness of van der Waals materials. This study investigates 3R-MoS_2 using various optical measurement techniques at room temperature and reveals apparent signal changes corresponding to different ferroelectric stacking orders and variations in layer count. Our findings demonstrate that fast optical mapping at room temperature is a reliable method for probing ferroelectric potential steps in 3R-stacked MoS_2 samples, thereby facilitating the identification of the ferroelectric configuration.

HL 24.10 Wed 12:00 POT/0081

Robust Orbital-Selective Flat Bands in Transition-Metal Oxychlorides — Xiangyu Luo[1], •Ludovica Zullo[2], Sahaj Patel[1], Dongjin Oh[1], Qian Song[1], Asish K. Kundu[3], Anil Rajapitamahuni[3], Elio Vescovo[3], Natalia Olszowska[4], Rafal Kurleto[4], Dawid Wutke[4], Giorgio Sangiovanni[2], and Riccardo Comin[1] — [1]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA — [2]Universität Würzburg, 97074 Würzburg, Germany, ct.qmat — [3]National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, USA — [4]Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Krakow, Poland

Flat electronic bands, which amplify electron correlations by quenching kinetic energy, provide an ideal foundation for exotic quantum phases. Here, we unveil an intrinsic orbital-selective flat-band mechanism in the van der Waals materials $NbOCl_2$ and $TaOCl_2$, directly observed by angle-resolved photoemission spectroscopy (ARPES) and understood through density functional theory (DFT) and Wannier analysis. Crucially, we experimentally demonstrate that this momentum-independent flat band exhibits remarkable robustness, surviving from the bulk crystal down to the few-layer limit at room temperature. Our theoretical analysis traces its origin to the hybridization between Nb-dz^2 orbital chains and the Lieb-like dx^2-y^2 sublattice, which is further reinforced by Peierls dimerization. Our findings uncover a new orbital-selective design principle for realizing flat bands in quantum materials.

HL 24.11 Wed 12:15 POT/0081

Tuning the Metal-to-Semiconductor Transition in Bilayer PtTe2 via Electric Field Control — •Sharieh Jamalzadeh Kheirabadi, Farzan Gity, Paul K.Hurley, and Lida Ansari — Tyndall National Institute, University College Cork, Cork, Ireland

Abstract: One effective method to induce a bandgap in graphene is applying a perpendicular electric field to its bilayer structure [1]. This process works by breaking the inversion symmetry of BL gra-phene with an external electric field, leading to electrostatic screening between the two layers and splitting the π and π^* bands that intersect at the Fermi level [2]. Platinum ditelluride (PtTe2) has garnered significant interest due to its unique physical and chemical properties [3,4]. PtTe2 retains its semi-metallic properties for thicknesses down to BL but transits to a semiconductor when re-duced to a monolayer due to the quantum confinement effect [5]. We demonstrate that a bandgap emerges in BL-PtTe2 when an electric field is applied perpendicular to the layers, ultimately trans-forming the system into a semiconductor. We have identified reliable critical electric fields within the range of 2-3 MV/cm to achieve a bandgap comparable to conventional semiconductors in BL-PtTe2. Further, we have investigated the effect of a vertical electric field on a BL-PtTe2 based field effect transistor using density functional theory (DFT) and non-equilibrium Green*s function (NEGF) methods. The results demonstrate device performance compatible with low-power require-ments for ION and IOFF, as projected in the IRDS 2028 roadmap [6].

HL 24.12 Wed 12:30 POT/0081

Circular Dichroism ARPES Reveals Orbital Chirality in Single-Layer TMDs — •Shubham Patel, Luke Pimlott, and Habib Rostami — Department of Physics, University of Bath, Claverton Down BA2 7AY, United Kingdom

The electron wavefunctions in momentum space are fundamental to understanding the microscopic physical properties of solids. Circular dichroism (CD), a key feature observable in angle-resolved photoemission spectroscopy (ARPES) [1]. Recent experimental investigations have indicated a direct relationship between CD-ARPES and the Berry curvature of electronic bands [2], motivating theoretical efforts to interpret CD within this framework. The Berry curvature-based approach fails to capture certain critical sign-reversal features near the time-reversal-invariant K(K') points. Moreover, this method lacks dependence on the photon energy of the incident light, as it is derived purely from the momentum-space wavefunction characteristics. In the present work, we adopt this plane wave approximation to compute CD-ARPES spectra and find excellent agreement with experimental observations. We solve tight-binding Hamiltonian for single-layer TMDs, and generalize the dipole matrix elements. This formalism successfully captures the sign-changing behavior of CD near the K(K') points, a feature absent in the Berry curvature approach, and provide a control on tunability of the dichroic response with the photon energy. Notably, our theoretical approach offers an alternative explanation that differs from

the Berry curvature-based framework.

[1] PRL 110, 216801 (2013) [2] PRL 121, 186401 (2018)