DS 7: 2D Materials and their Heterostructures III

Time: Wednesday 9:30–11:45 Location: A 053

DS 7.1 Wed 9:30 A 053

Two-dimensional platinum chalcogenides: controlling stoichiometry for electronic applications — •Mahdi Ghorbani-Asl and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany.

Among layered materials, platinum chalcogenides have received great attention due to their peculiar physical properties. The strong layer-dependent electronic properties cause the opening of a band gap in monolayer $PtTe_2$, while the system otherwise is (semi)metallic. Here we show that starting with $PtTe_2$ films, other compositions such as Pt_3Te_4 and Pt_2Te_2 can be obtained by a postgrowth desorption of tellurium or vapor-deposited Pt atoms. The experiments combined with DFT calculations provide insights into these transformation mechanisms and the stabilization of the new phases. The partially converted monolayer flakes exhibit $PtTe_2$-Pt_2Te_2 heterojunctions, which enable the formation of the in-plane semiconductor-metal interface. We further studied the electronic structure of edges and point defects in $PtSe_2$ monolayer where metallic 1D states with spin-polarized bands were found. In addition to stoichiometry, combining different Pt-chalcogenides in the form of vertical heterostructures provides an additional degree of engineering of materials properties. Our results showed the variation of the interlayer interaction within the moiré structure locally modulates the electronic structure of $PtSe_2/PtTe_2$ heterostructures.

DS 7.2 Wed 9:45 A 053

Classification of layered chalcogenides: explaining their mineral diversity in the Earth's crust — •Alexander Kiehn[1], Carl-Friedrich Schön[2], Christian Stenz[2], Sebastian Gruner[2], Jan Köttgen[2], Jean-Yves Raty[3], and Matthias Wuttig[1,2] — [1]PGI 10, Forschungszentrum Jülich; Johnen-Straße, 52428 Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University; Sommerfeldstraße 14, 52056 Aachen, Germany — [3]CESAM, Université de Liège; Quartier Agora, Allée du six Août 19, 4000 Liège, Belgium

Layered or 2D chalcogenides are a material class with exceptional properties enabling manifold applications. Using quantum-chemical calculations, these materials can be classified into three families based on the distance between layers as well as the translation energy parallel to these layers. Containing many TMDCs, the largest group of layered chalcogenides forms van der Waals bonds across the gaps, which are characterized by large atomic spacings, small translation energies and weak interlayer bonding. Conversely, two other groups are identified by shorter interlayer gaps, larger translation energies and significantly stronger interlayer coupling. For several compounds, like Bi2Te3, these properties can be attributed to their special bonding mechanism. Notably, when combining compatible layer types into varying stacks, this large coupling allows for an energy hierarchy of interlayer bonding. This explains the rich phase diagrams of heavy p-block elements, like Sb, As, Bi and Te, and is also mirrored in their anomalously high mineral diversity. The evidence for strong interlayer coupling is supported by electron microscopy and laser-assisted bond-rupture experiments.

DS 7.3 Wed 10:00 A 053

Misfit Layer Compounds as Ultratunable Field Effect Transistors: From Charge Transfer Control to Emergent Superconductivity — •Ludovica Zullo[1,2], Giovanni Marini[1], Tristan Cren[2], and Matteo Calandra[1,2,3] — [1]Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy — [2]Sorbonne Université, CNRS, Institut des Nanosciences de Paris (INSP), UMR7588, F-75252 Paris, France — [3]Graphene Labs, Fondazione Istituto Italiano di Tecnologia, Via Morego, I-16163 Genova, Italy

Misfit layer compounds (MCLs) are heterostructures composed of rocksalts units stacked with few layers transition metal dichalcogenides (TMDs) [1]. Because of the lattice mismatch and chemical bonding between constituents, bulk MLCs behave similarly to mono and bi layer TMDs, making it quasi-2D systems. In this work [2], by means of density functional theory, we show that misfits behave as a periodic arrangement of ultra-tunable field effect transistors with 2D features. We demonstrate how the charge injection into the TMD layers can be controlled by the chemistry of the rocksalt which always acts as electron donor. Finally, we establish a strategy to design emergent superconductivity and demonstrate its applicability in $(LaSe)_{1.27}(SnSe_2)_2$, showing that superconductivity can emerge in MLCs formed by assembling non-superconducting rocksalts and TMDs.

[1] Gerrit Wiegers, Progress in Solid State Chemistry 24, 1 (1996)
[2] Ludovica Zullo, Giovanni Marini, Tristan Cren, Matteo Calandra Nano Lett. 2023, 23, 14, 6658-6663 (2023)

DS 7.4 Wed 10:15 A 053

Direct visualization of stacking-selective self-intercalation in epitaxial $Nb_{1+x}Se_2$ films — Hongguang Wang[1], •Jiawei Zhang[1], Chen Shen[2], Chao Yang[1], Kathrin Küster[1], Ulrich Starke[1], Hongbin Zhang[2], Dennis Huang[1], Peter A. van Aken[1], and Hidenori Takagi[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Department of Materials and Earth Sciences, Technical University of Darmstadt, 64289 Darmstadt, Germany

Two-dimensional (2D) van der Waals (vdW) materials are particularly intriguing due to the rich tuning possibilities offered by stacking 2D layers or introducing intercalants into the vdW gaps. However, current knowledge of the interplay between stacking polytypes and intercalation is limited by macroscopically averaged probes. Here, using atomic-resolution electron energy-loss spectroscopy in a scanning transmission electron microscope, we directly visualize a stacking-selective self-intercalation phenomenon in the transition-metal dichalcogenide (TMDC) material $Nb_{1+x}Se_2$: In epitaxial $Nb_{1+x}Se_2$ films with both the parent 180° stacking and additional 0°-stacked phases, the excess Nb atoms are predominantly found between the 180°-stacked layers. The 0°-stacked layers arise as a means of staggering the intercalants, *i.e.*, to increase their interlayer separation, rather than to accommodate the intercalants themselves, as has been previously suggested. Our results not only provide an updated microscopic understanding of $Nb_{1+x}Se_2$, but also prospects for engineering the functionality of TMDCs via stacking-selective self-intercalation.

15 min. break

DS 7.5 Wed 10:45 A 053

Nontrivial magnetic helical states and electric polarization in NiI_2 monolayer — •Juraj Mnich[1] and Martin Gmitra[1,2] — [1]Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia — [2]Institute of Experimental Physics, Slovak Academy of Sciences, 04001 Košice, Slovakia

A monolayer of NiI_2 enriches a small group of 2D multiferroic materials possessing unique magnetic and electric polarization properties. Trigonal crystal symmetry and the interplay between spatially dependent ferromagnetic and antiferromagnetic exchange interactions, along with strong spin-orbit coupling, give rise to complex helical magnetic states. The helical state can be described by a wave propagation vector and a plane in which magnetic moments rotate. We studied several magnetic helical states using first-principles calculations. We found that the alignment of magnetic moments gives rise to unexpected electric polarization for a proper screw helical state. We also studied the interplay between the helical states and electric polarization in the NiI_2 bilayer and we speculate that an in-plane bias voltage can induce rotation of the helical state via spin-transfer torque, dragging its phase and switching the wave propagation vector, reflecting in electric polarization reversal.

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DS 7.6 Wed 11:00 A 053

Electronic structure of intercalated α-$NbSi_2N_4$ and α-$TaSi_2N_4$ monolayers and their van der Waals heterostructures — •Timon Moško[1] and Martin Gmitra[1,2] — [1]Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia — [2]Juraj Mnich Institute of Experimental Physics, Slovak Academy of Sciences, 04001 Košice, Slovakia

Recent DFT studies of monolayer materials promote intercalated MA_2Z_4 monolayers as versatile atomically thin materials with a wide spectrum of physical properties. In the talk, we present a first-

principles study of the electronic structure of α-$NbSi_2N_4$ and α-$TaSi_2N_4$ monolayers, as well as their heterostructure. We investigate mechanical stability, charge density wave formation, electronic susceptibility, and magnetic order. We found that the Hubbard on-site on metallic atoms M drives the α-$NbSi_2N_4$ from a magnetic conductor to a magnetic insulator and α-$TaSi_2N_4$ from a non-magnetic Eliashberg superconductor to a magnetic insulator. Magnetic ground state properties were analyzed using a classical Heisenberg model, providing insights into exchange integrals, magnetocrystalline anisotropy, and critical transition temperatures. Proximity-induced effects in α-$NbSi_2N_4$ / α-$TaSi_2N_4$ heterostructure uncover lead to the doping effect and emergence of the narrow Ta d_{z^2} hole pocket at the Brillouin zone center susceptible to suggesting its potential as a hybrid system for controlling spin and thermal transport under a transverse electric field.

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DS 7.7 Wed 11:15 A 053

Quasiparticle Interference patterns of monolayer $NbSe_2$, an Ising superconductor with Rashba spin-orbit coupling — •Jozef Haniš[1], Marko Milivojević[2,3], and Martin Gmitra[1,4] — [1]Institute of Experimental Physics, Slovak Academy of Sciences, 04001 Košice, Slovakia — [2]Institute of Informatics, Slovak Academy of Sciences, 84507 Bratislava, Slovakia — [3]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [4]Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia

A monolayer of $NbSe_2$ is a 2D superconductor with unconventional Ising pairing that sustains tremendous in-plane magnetic fields. In a realistic setup, the presence of the substrate triggers the Rashba spin-orbit coupling in $NbSe_2$ and an in-plane spin texture in the superconducting material. It was experimentally suggested that such a system can host both nodal and nematic superconductivity, motivating us to theoretically construct all the possible types of singlet and triplet superconducting pairings allowed. Furthermore, we calculate the quasiparticle interference (QPI) patterns in the limit of a single scalar impurity. We found pronounced differences in the QPI patterns of the superconducting pairing functions constructed using the group-theoretical approach, suggesting that the QPI spectrum analysis can provide valuable insights into the potential understanding of the unconventional pairing when confronted with the scanning tunneling spectroscopy measurements.

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DS 7.8 Wed 11:30 A 053

Visible-Light-Active 2D Single-Layered g-C_3N_4-TiO_2 Thin Film Photocatalysis — •Narmina O. Balayeva[1,2], Bowei Zhan[1,2], Yevhenii Havryliuk[1,2], Oleksandr Selyshchev[1,2], and Dietrich R.T. Zahn[1,2] — [1]Institute of Physics, TU Chemnitz, Reichenhainer Str. 70 — [2]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), TU Chemnitz, Rosenbergstr. 6

Recently, the interest in the application of atomically thin 2D "graphene-like" layered graphitic carbon nitride (g-C_3N_4) for visible-light efficient photocatalysis has significantly increased. This work demonstrates the fabrication of thin film heterostructures of single-layered g-C_3N_4 (SLGCN) and the anatase TiO_2. After obtaining SLGCN from base-assisted exfoliation of bulk g-C_3N_4, the films were prepared using spray coating with 1, 3, and 5 cycles on p-type Si(100) substrates. Subsequently, a colloidal TiO_2 solution was deposited using spin coating and annealed at 500 °C to form the anatase polymorph. Secondly, the powder of SLGCN was mixed with the colloidal TiO_2 solution at different relative weight percentages (5-50 wt%) and deposited using spin coating followed by the same annealing procedure. The morphology, structural, and optical properties of SLGCN and SLGCN-TiO_2 are characterized by XRD, AFM, SEM, and spectroscopic techniques such as UV-vis, Raman, FTIR, and ellipsometry. Finally, the photocatalytic degradation of acetone and CO_2 reduction was studied using an FTIR-based gas photo-reactor chamber equipped with 1 mW/cm^2 LED with different wavelengths.