O 29: Poster: 2D Materials

Time: Tuesday 12:30–14:30 Location: Poster A

O 29.1 Tue 12:30 Poster A

Precision in Growth: Knudsen Cells and Solution-Coated Precursors Revolutionize TMDC Synthesis by CVD — •Thomas Aquinas Pobi, Osamah Kharsah, Jonah von Kuczkowski, and Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik und CENIDE, Duisburg,Germany

Chemical Vapor Deposition (CVD) stands out as a reliable technique for synthesizing transition metal dichalcogenides (TMDCs) like MoS2 and WS2 . However, the process's susceptibility to minor variations in growth parameters often hampers reproducibility. This study introduces a novel approach utilizing a combination of Knudsen cells and a solution-based, spin-coated precursor to address this challenge. By ensuring a constant and sustainable chalcone supply, this method not only overcomes reproducibility issues but also enhances the spatial distribution of the precursor. The results demonstrate a successful transition from diffusion-limited growth to attachment-limited growth, marking a significant advancement in TMDC synthesis.

O 29.2 Tue 12:30 Poster A

h-BN in the Making: The Surface Chemistry of Borazine on Rh(111) — •Eva Marie Freiberger[1], Fabian Düll[1], Phiona Bachmann[1], Johann Steinhauer[1], Hans-Peter Steinrück[1], and Christian Papp[1,2] — [1]FAU Erlangen-Nürnberg, Erlangen, Germany — [2]FU Berlin, Berlin, Germany

The intriguing properties of two-dimensional materials (2DM) gave rise to a vivid research field. One of the most-studied representatives of this class is hexagonal boron nitride (h-BN). In ultra-high vacuum (UHV), h-BN can be grown on a metal support via chemical vapor deposition (CVD) using suitable precursors, such as ammonia borane or borazine. h-BN grown on a lattice-mismatched substrate undergoes a buckling, which is, in the case of Rh(111), referred to as nanomesh.

In this UHV study, we investigated the evolution of the h-BN nanomesh from borazine on Rh(111) using synchrotron radiation-based high-resolution X-ray photoelectron spectroscopy (XPS). The adsorption of borazine at 130 K was followed in situ, showing that borazine adsorbs mainly as an intact molecule. By studying borazine on Rh(111) with NEXAFS, we were able to identify a flat-lying adsorption geometry. For a better understanding regarding the formation of h-BN, the thermally-induced reaction of borazine on Rh(111) was investigated by temperature-programmed XPS. We find that borazine multilayers already desorb below 200 K. At 300 K, dehydrogenation of the remaining monolayer occurs, and boron nitride starts to grow in a disordered fashion. Above 600 K, the formation of the nanomesh sets in and, at about 1100 K, the conversion to h-BN is complete.

O 29.3 Tue 12:30 Poster A

2D porous fantrip network on calcite (10.4) as a starting point for on-surface synthesis — •Lea Klausfering[1], Lukas Höltkemeier[1], Ralf Bechstein[1], Markus Lackinger[2], and Angelika Kühnle[1] — [1]Physical Chemistry I, Bielefeld University, 33615 Bielefeld, Germany — [2]Deutsches Museum, 80538 Munich, Germany

Triptycen anthracene derivatives have proven to be suitable molecules for two-dimensional polymers. For example the deposition on crystal surfaces under ultra-high vacuum (UHV) conditions is possible. Under UHV conditions, the fluorinated anthracene triptycene (fantrip) molecule was investigated on graphite (0001) [1] and Au (111) [2] surfaces. However, in both cases, a porous Fantrip network could only be obtained when passivating the surface prior to molecule deposition. Otherwise, the molecules did not lie perpendicular with all three anthracene blades with respect to the surface as desired, but parallel with two anthracene blades and upright with one anthracene blade. The passivation reduces the molecule-surface interaction. Here, we show that the porous fantrip network can be achieved without surface passivation when using the (10.4) surface of the bulk insulator calcite. The resulting network provides a good starting point for [4+4]-photocycloaddition on the surface to generate a two-dimensional polymer.

[1] L. Grossmann et al., Nature Chemistry, 2021, 13, 730-736.

[2] L. Grossmann et al., Angew. Chem. Int. Ed., 2022, 134, e202201044.

O 29.4 Tue 12:30 Poster A

Growth of two-dimensional hexagonal β-GeSe on Au(111) — •Dina Wilks, Veronika Blecker, Marina Hammer, Muhammad Ali Martuza, Paulus Aleksa, and Carsten Busse — Department Physik, Universität Siegen, Walter-Flex-Straße 3, 57072 Siegen

Two-dimensional group-IV monochalcogenides (general form MX with M=Sn, Ge; X=S, Se, Te) have great potential in nanotechnology due to their versatility. Theory predicts several polymorphs of these materials. For GeSe none of these have been confirmed experimentally, unlike SnSe, SnS, and SnTe.
We report the first experimental realization of β-GeSe which has a corrugated honeycomb structure. The monolayers are prepared under highly controlled conditions (molecular beam epitaxy from GeSe powder on a single crystalline Au(111) substrate under ultra-high vacuum (UHV) conditions). We find a temperature window for self-limiting monolayer growth. Low-energy electron diffraction (LEED) reveals a (5×5) superstructure with respect to Au(111). For sub-monolayer coverage, we find orientational disorder while the full layer is highly aligned with respect to the sample. Scanning tunneling microscopy (STM) shows that a superstructure unit cell contains (4×4) β-GeSe unit cells. The Au(111) herringbone reconstruction is lifted under the MX-monolayer.

O 29.5 Tue 12:30 Poster A

Facile chemical vapor deposition growth of transition metal dichalcogenide alloy lateral heterostructures for electronic and optoelectronic applications — Seung Heon Han[1], Gia Quyet Ngo[2], Moritz Quincke[3], Emad Najafidehaghani[1], •Christof Neumann[1], Uwe Hübner[4], Ute Kaiser[3], Falk Eilenberger[2,5], Antony George[1], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Institute of Applied Physics, Abbe Center of Photonics, Friedrich Schiller University Jena, 07745 Jena — [3]Central Facility of Electron Microscopy, Ulm University, 89081 Ulm — [4]Leibniz Institute of Photonic Technology (IPHT), 07745 Jena — [5]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, 07745 Jena

Lateral heterostructures (LH) of monolayer transition metal dichalcogenides (TMDs) such as MoS_2, WSe_2 are known for their high potential for the integration in ultrathin device technology as p-n junction diodes and photodetectors. While the properties of pure TMDs are noteworthy, the development of alloy TMDs (e.g., $Mo_xW_{(1-x)}S_2$ etc.) adds a new dimension to the research on 2D semiconductors. Alloy TMDs allow for the fine-tuning of their intrinsic electronic properties, thereby expanding the spectrum of potential applications. Here we present the growth of monolayer alloy LHs by CVD employing liquid precursors of transition metals. We characterized the synthesized material by AFM, Raman spectroscopy, HRTEM, as well as, PL spectroscopy and studied their performance in optoelectronic devices.

O 29.6 Tue 12:30 Poster A

Modifications of the Au(111) reconstruction induced by the adsorption of P_2 and its role for the growth of blue-phosphorus. — •Morris Mühlpointner and Moritz Sokolowski — Clausius Institute for Physical and Theoretical Chemistry of the University of Bonn, Wegelerstr. 12, 53115, Bonn Germany

The adsorption of phosphorus on the Au(111) surface has been studied under the aim to grow a two-dimensional "blue-phosphorus" (bP) structure, which is analogous to graphene. Furthermore, phosphorus adsorption has been shown to alter the structure of the Au(111) reconstruction from the herringbone reconstruction to a "trigon reconstruction" (TR) [1].

In the present work, we investigated the structure of the TR for increasing bP coverages using high-resolution spot-profile analyzing low-energy electron diffraction (SPA-LEED). We observed the TR prior to bP film growth with a highly-ordered structure. At higher P-coverages, patches of the bP structure and the TR coexist. With time, the structure of the TR distorts and forms disordered patches of Au(111) surface that exhibit low P-coverages. Further insight was obtained by temperature programmed desorption (TPD) spectra, which show a zero-order desorption peak, regardless of the starting coverage. We propose that this zero-order desorption peak can be explained by a phase-equilibrium.
[1] ACS Nano **14**, 3687-3695, 2020 .

This work was supported by the DFG through the research training group 2591.

O 29.7 Tue 12:30 Poster A

Electronic Fingerprints of Platinum Surface Tellurides and $\mathrm{Pt_xTe_y}$ Films on Pt(111)

— •Isabella Stollberg, Andreas Raabgrund, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

For the synthesis of transition metal dichalcogenides, in general two approaches can be utilized: evaporating the metal and the chalcogenide on a suitable substrate [1] or directly depositing only the chalcogenide on a desired metal substrate. We investigated by STM, STS, and DFT the properties of $\mathrm{Pt_xTe_y}$ films on Pt(111) that are synthesized according to the latter approach. Depending on Te content, a (3×3) and (10×10) surface telluride structure are found, followed by the growth of $\mathrm{Pt_2Te_2}$ and $\mathrm{PtTe_2}$ [2].

Applying STS measurements we found characteristic features on the respective structures which can be used as fingerprints for identification. By comparison with DFT calculations we attribute the STS features to electronic states within the telluride films. Additionally, we determined the work function differences probing field emission resonances. We find that the (10×10) surface telluride has the lowest but $\mathrm{Pt_2Te_2}$ and $\mathrm{PtTe_2}$ have very similar work functions.

[1] K. Lasek et al., Nano Lett. **22**, 23 (2022)

[2] T. Kißlinger et al., Phys. Rev. B **108**, 205412 (2023)

O 29.8 Tue 12:30 Poster A

Properties and modification of antimonene on Ag(111)

— •Felix Otto, Leon Bojunga, Christian Haberland, Jonas Brandhoff, Maximilian Schaal, Marco Gruenewald, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

The search for novel two-dimensional (2D) materials with beneficial structural, electronic or optical properties is of great interest for many researchers as well as, to an increasing extend, for industry. For this reason, we investigate the properties of antimonene on Ag(111) with respect to the adsorption of organic molecules as well as atoms.

These were in a first part investigated by using the organic molecule 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA), which has well-known properties and serves as a sensor for the decoupling properties of the Sb-films. For this, differential reflectance spectroscopy (DRS) together with photoelectron spectroscopy (PES) was performed. This yields a classification of the PTCDA-Sb interaction in comparison to other substrates.

In a second part we modified the Sb on Ag(111) system by the deposition of phosphorous in order to grow an inorganic 2D heterolayers. However, we will show by low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) measurements that phosphorous did not form ordered films on top of Sb. Instead, our structural and electronic characterization revealed that P is able to form an ordered intermediate layer below α-antimonene.

O 29.9 Tue 12:30 Poster A

Epitaxial growth and properties of sub-monolayer to multilayer $\mathrm{FeBr_2}$ on Au(111)

— •S. E. Hadjadj[1], C. González-Orellana[2], J. Lawrence[3], D. Bikaljević[4,5], M. Peña-Díaz[2], P. Gargiani[6], L. Aballe[6], J. Naumann[7], M. Ángel Niño[6], M. Foerster[6], S. Ruiz-Gómez[8], S. Thakur[1], I. Kumberg[1], J. Taylor[9,10], J. Hayes[1], J. Torres[1], C. Luo[9,10], F. Radu[9], D. G. de Oteyza[3,11], W. Kuch[1], J. I. Pascual[4,12], C. Rogero[2,3], and M. Ilyn[2] — [1]Freie Universität Berlin, Experimentalphysik, Germany — [2]Centro de Física de Materiales, Donostia, Spain — [3]Donostia International Physics Center, Spain — [4]CIC nanoGUNE-BRTA, Donostia, Spain — [5]Institute of Physical Chemistry, University of Innsbruck, Austria — [6]ALBA Synchrotron Light Source, Spain — [7]Freie Universität Berlin, Dahlem Center for Complex Quantum Systems, Germany — [8]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [9]HZB, Germany — [10]Physik, Technische Universität München, Germany — [11]Nanomaterials and Nanotechnology Research Center (CINN), Oviedo, Spain — [12]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

We characterized the properties of the van-der-Waals material $\mathrm{FeBr_2}$ on Au(111). The investigation via STM and LEED reveals a dominant superstructure for the first layer, which changes for the second layer. The characterization by XPS and XAS shows that the chemical composition does not change for different coverages. The magnetic characterization by XMCD reveals that the magnetization at 6 T increases during the transition from first to the second monolayer.

O 29.10 Tue 12:30 Poster A

The Effect of $\mathrm{WS_2}$-$\mathrm{Cu_2O}$ for the Optimization of a $\mathrm{WS_2}$-based LED

— •Jonah von Kuczkowski[1], Osamah Kharsah[1], Leon Daniel[1], Stephan Sleziona[1], Denys Vidish[2], Kevin Musselman[2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, Fakultät für Physik und CENIDE, Duisburg, Germany — [2]University of Waterloo, Mechanical and Mechatronics Engineering, Waterloo, Canada

Scalable 2D material based LEDs have been the subject of many recent works. Tungsten disulfide ($\mathrm{WS_2}$) emerges as a potential active material in such LEDs, based on its direct band gap, high stability and strong photoluminescence. Copper oxide ($\mathrm{Cu_2O}$) on the other hand, a p-type semiconductor, can function as the electron-transport layer. This study investigates the interaction between $\mathrm{WS_2}$ and $\mathrm{Cu_2O}$ within the framework of the LED. Different characterization techniques, including (low-temperature) PL, Raman spectroscopy for optoelectronic interaction and various electrical transport measurements are employed to map out the benefits and limitations of using $\mathrm{Cu_2O}$ in the $\mathrm{WS_2}$ based LED.

O 29.11 Tue 12:30 Poster A

Photoluminescence upconversion in monolayer $\mathrm{WSe_2}$ activated by plasmonic cavities through resonant excitation of dark excitons

— •Niclas S. Mueller[1,2], Rakesh Arul[1], Gyeongwon Kang[1], Ashley P. Saunders[3], Amalya C. Johnson[3], Ana Sánchez-Iglesias[4], Shu Hu[1], Lukas A. Jakob[1], Jonathan Bar-David[1], Bart de Nijs[1], Luis M. Liz-Marzán[4], Fang Liu[3], and Jeremy J. Baumberg[1] — [1]NanoPhotonics Centre, University of Cambridge, UK — [2]Present address: Fritz Haber Institute of the Max Planck Society Berlin, Germany — [3]Department of Chemistry, Stanford University, USA — [4]CIC biomaGUNE, Donostia-San Sebastián, Spain

Anti-Stokes photoluminescence (PL) is light emission at a higher photon energy than the excitation, with applications in optical cooling, lasing, and the detection of infrared light. Here, we show how plasmonic nano-cavities activate anti-Stokes PL in $\mathrm{WSe_2}$ monolayers through resonant excitation of a dark exciton at room temperature. The optical near-fields of the plasmonic cavities excite the out-of-plane transition dipole of the dark exciton, leading to light emission from the bright exciton at higher energy. Through statistical measurements on hundreds of plasmonic cavities, we show that coupling to the dark exciton leads to a near hundred-fold enhancement of the upconverted PL intensity. We further demonstrate a selective and reversible switching of the upconverted PL via electrochemical gating.

[1] Mueller et al. Nat. Commun. 14, 5726 (2023)

O 29.12 Tue 12:30 Poster A

Characterization of single-layer NbSe2

— •Caroline Firschke[1], Verena Caspari[1], Jean-Maxime Schlachter[2,3], Matthieu Jamet[2,3], Clemens B. Winkelmann[2,3], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Germany — [2]Université Grenoble Alpes, France — [3]CEA Grenoble, France

A single layer of the superconductor NbSe2 exhibits different properties than its bulk counterpart due to its reduced dimensionality. For example, strong spin-orbit coupling combined with the lack of inversion symmetry locks electrons with opposite spin and momenta, resulting in an increased in-plane critical field.

Here, we use scanning tunneling microscopy (STM) at 1.1K to characterize single-layer NbSe2-islands on a bi-layer graphene on SiC, grown by molecular beam epitaxy. These samples had been capped with Se for transport from the growth chamber to the STM, which we remove by heating under ultra-high vacuum conditions. Although this procedure does not lead to atomically clean layers, we detect a superconducting gap and low-energy excitations outside of it, interpreted as Legget modes that are in agreement with the work by W. Wan et al. [1].

[1] Wen Wan et al. "Observation of Superconducting Collective Modes from Competing Pairing Instabilities in Single-Layer NbSe2". Adv. Mat. 34, 2206078 (2022)

O 29.13 Tue 12:30 Poster A

Machine learning angle resolved photoemission spectroscopy spectrum of transition metal dichalchogenide materials

— •Ridha Eddhib and Jan Minar — New Technologies - Research Centre, University of West Bohemia, 301 00 Pilsen, Czech Republic.

Predicting material properties through machine learning necessitates the development of a specific descriptor, serving as a distinctive fingerprint for the desired properties. This descriptor becomes the input for the machine learning model, typically crafted by leveraging atomic structures as the primary source of information. Fortunately, there already exists a comprehensive repository of descriptors for encoding atomic structures. Our research focuses on the challenge of representing the mapped quantum states angularly resolved for photoemitted electrons in a solid, specifically targeting machine learning applications for state-specific electronic properties. In this context, we introduce a descriptor for Angle-Resolved Photoemission Spectroscopy (ARPES) based on the energy decomposed operator matrix elements (ENDOME) fingerprints[1]. Notably, our work sheds light on a significant limitation present in various Density Functional Theory (DFT)codes,they commonly lack the capability to directly compute ARPES spectra. Our efforts not only address this critical gap but also stand as a pioneering effort to pave the way for accurate estimates of ARPES spectra contributing significantly to the advancement of machine learning methodologies applied to materials science.[1] Knøsgaard, N. R., & Thygesen, K. S. (2022). Nature Communications, 13(1),468.

O 29.14 Tue 12:30 Poster A

Floquet Engineering in TMDs using short pulsed lasers — •Alejandro Sebastián Gómez[1], Yuriko Baba[2], Rafael A. Molina[1], and Francisco Domínguez-Adame[3] — [1]Instituto de Estructura de la Materia, IEM-CSIC, Madrid, Spain — [2]Universidad Autónoma de Madrid, Madrid, Spain — [3]GISC, Universidad Complutense de Madrid, Madrid, Spain

This work focuses on the use of pulsed lasers to manipulate certain properties of Transition Metal Dichalcogenides (TMDs), a type of two-dimensional material [1] . For this purpose, the well-known method of Floquet engineering is employed, capable of describing quantum systems with a perfectly periodic driven external field. The aim is to understand how effectively Floquet theory can be applied to non-periodic pulses such as those in pulsed lasers. To achieve this, the we employ the t-t' formalism technique [2], offering an interesting method for analyzing short pulses.

[1] Liu, G. B., Xiao, D., Yao, Y., Xu, X., & Yao, W. (2015). Electronic structures and theoretical modelling of two-dimensional group-VIB transition metal dichalcogenides. Chemical Society Reviews, 44(9), 2643-2663. [2] Ikeda, T. N., Tanaka, S., & Kayanuma, Y. (2022). Floquet-Landau-Zener interferometry: Usefulness of the Floquet theory in pulse-laser-driven systems. Physical Review Research, 4(3), 033075.

O 29.15 Tue 12:30 Poster A

Local Work Function Modulation of Hexagonal Boron Nitride on Pt(110) — •Marco Thaler, Matthias Zeilerbauer, and Laerte Patera — University of Innsbruck, Austria

Hexagonal boron nitride (h-BN) offers a wide band gap, high thermal stability and low chemical reactivity and therefore has emerged as a promising candidate to serve as an ultra thin layer for the deposition and decoupling of organic molecules on surfaces. Remarkably, on the incommensurate Pt(110) surface, h-BN can be grown as a large-area single-domain monolayer of excellent quality. The lattice mismatch between the hexagonal adlayer and the platinum substrate leads to the formation of a distinctive moiré pattern. Using field emission resonance spectroscopy (FERS), a spatial modulation of the local work function can be observed depending on which moiré region is examined. Upon room temperature deposition of 5,10,15,20-Tetrakis(4-aminophenyl)porphyrin (Co-TAPP), the porphyrins arrange into clusters occupying a variety of adsorption sites of the h-BN/Pt(110) unit cell. With the help of scanning tunneling spectroscopy a site-specific shift of the Co-TAPP states is observed, which can be associated to the local work function differences of the underlying substrate. This shows that Co-TAPP can act as an effective probe to study the work function landscape of our system.

O 29.16 Tue 12:30 Poster A

Can we disentangle the electronic contribution from the surface corrugation of the charge density wave in 2H-NbSe2? — •Nikhil Seeja Sivakumar[1], Joost Aretz[1], Sebastian Scherb[1], Marion van Midden Mavric[2], Nora Huijgen[1], Umut Kamber[3], Daniel Wegner[1], Alexander Ako Khajetoorians[1], Malte Rösner[1], and Nadine Hauptmann[1] — [1]Institute of Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Condensed matter physics department, Jozef Stefan Institute, Ljubljana, Slovenia — [3]Department of Physics, Princeton University, USA

A charge density wave (CDW) is a collective phenomenon present in many quantum materials. Currently, the formation mechanism of the CDW in 2H-NbSe2 is understood to originate from momentum and orbital dependent electron phonon coupling. Still, there are open questions regarding the involved bands and the role of Se atoms in the formation of the CDW. Here we utilize combined Scanning Tunnelling Microscopy (STM) and non-contact Atomic Force Microscopy (nc-AFM) to independently characterize the geometric as well as the electronic structure of the CDW in 2H-NbSe2. Distance-dependent current and frequency shift images reveal a different evolution of the relative contrast of the atomic and CDW periodicities. We utilize Scanning Tunnelling Spectroscopy to characterize the electronic structure close to the Fermi level. We compare the experimental results with ab-initio calculations of the energy and momentum-resolved charge density.

O 29.17 Tue 12:30 Poster A

Exploring Excitonic Dispersions in 2D WS$_2$ through Spatially Resolved Electron Energy Loss Spectroscopy — •Max Bergmann, Jürgen Belz, Oliver Massmeyer, Badrosadat Ojaghi Dogahe, Robin Günkel, Johannes Glowatzki, Andreas Beyer, Stefan Wippermann, and Kerstin Volz — Material Sciences Center and Department of Physics, Philipps-Universität Marburg, Germany

Two-dimensional transition metal dichalcogenides have attracted considerable attention in materials science, particularly in the field of valleytronics, due to their unique indirect-to-direct bandgap transition and enhanced quantum efficiency in the monolayer limit. In this study we use a monochromated scanning transmission electron microscope to measure the electron energy loss spectrum of WS$_2$ providing nanometer-scale spatial resolution. The measurements reveal redshifts of the excitonic excitations due to a change in the WS$_2$ layer number for both the excitons residing at the K-point of the band structure and excitonic features stemming from more diverse excitations at points between Γ and K. To assess the origin of these excitations, theoretical investigations, namely density functional theory with Bethe-Salpeter equations on top, were used. This comprehensive investigation provides valuable insights into the excitonic properties of WS$_2$ across different layer configurations, highlighting in particular the dispersion of excitons with respect to changes in layer number.

O 29.18 Tue 12:30 Poster A

Electronic properties of a magnetic semiconductor: V-doped WSe$_2$ — •Jana Kähler[1,2], Sinja H. Weychardt[1,2], Florian K. Diekmann[1,2], Matthias Kalläne[1,2], and Kai Rossnagel[1,2] — [1]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics is proposed as an energy efficient alternative to conventional electronics with a wide range of applications, e.g., in the field of quantum computing. To realize efficient spin transport properties, magnetic semiconductors with a Curie temperature around room temperature and the ability to switch the magnetic order by electrical gating are promising candidates. The vanadium-doped layered transition metal dichalcogenide $2H$-WSe$_2$, which is characterized by strong spin-orbit coupling, a homogeneous magnetic doping distribution up to doping levels of a few percent, and the prediction of gate tunability, is a very promising candidate. However, many open questions remain regarding the electronic functionality.

Here, we present first results on the electronic transport properties and the momentum-resolved electronic structure of V-doped WSe$_2$ in comparison to pristine bulk samples. The samples were grown in our laboratory by chemical vapor transport and with different doping concentrations. Future magnetic structure investigations such as X-ray magnetic circular dichroism and spin- and momentum-resolved photoemission spectroscopy are discussed.

O 29.19 Tue 12:30 Poster A

Ultrafast spin dynamics and their layer-specific spin polarization of conduction band electrons in pristine and Cs-doped WSe$_2$ — •Sebastian Hedwig, Gregor Zinke, Benito Arnoldi, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany

Layered 2D Van-der-Waals systems are a highly intriguing class of low-dimensional materials with promising spin functionalities for future nanoscale spintronic applications. A particularly interesting member of this class of materials are WSe_2 bulk crystals with their hidden spin polarization. These centrosymmetric bulk crystals exhibit an overall spin degenerate band structure while each individual layer is characterized by spin-split valence bands. We conduct time-, spin- and angle-resolved photoemission experiments to study the optically excited spin carrier dynamics at the K- and Σ-points of WSe_2. The high surface sensitivity of the photoemission experiments allows us to disentangle the spin polarization of the bands in the first WSe_2 layer. After an initial spin-selective excitation at the K-point, which depends on the pump light polarization [1], we observe a subsequent intraband scattering from the K- to the Σ-point of the WSe_2 conduction band. This intraband scattering leads to a time-dependent change in the spin polarization of the carriers at the Σ-point. We compare the optically generated spin-dependent carrier population at the Σ-point with that one of Cs-doped WSe_2 for which the conduction band valley at the Σ-point is fully occupied. [1] Phys. Rev. Lett. 117, 277201 (2016)

O 29.20 Tue 12:30 Poster A

Electronic structure of intercalated stacks of two-dimensional crystals — Franziska Rauh and •Sabine Körbel — Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena, Germany

Layered Van-der-Waals crystals with their atomic sheets separated by several Ångström, such as stacks of two-dimensional transition-metal dichalcogenides, allow for intercalation with elements or molecules. Here we consider intercalation as a means to manipulate the electronic structure of the layered crystal. We attempt to turn a metal into an insulator, and to create a stair-case band alignment in another insulator. We determine the electronic structure of the intercalated crystals from first principles using density-functional theory.

O 29.21 Tue 12:30 Poster A

Modelling ARPES matrix elements in a 2D van-der-Waals ferromagnet — •Tania Mukherjee[1,2], Lawson Lloyd[2], Samuel Beaulieu[3], Michael Schuler[4], Jyoti Krishna[5], Túlio de Castro[2], Shuo Dong[6], Victoria Taylor[2], Yoav William Windsor[1,2], Martin Wolf[2], Laurenz Rettig[2], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1,2] — [1]Technische Universität Berlin, Berlin, Germany — [2]Fritz-Haber-Institute of the Max Planck Society — [3]University of Bordeaux, France — [4]PSI, Villigen, Switzerland — [5]Freie Universität Berlin, Berlin, Germany — [6]Beijing National Laboratory for Condensed Matter Physics, Beijing, China

Recent discoveries of 2D materials with intrinsic ferromagnetic ordering show great potential for new spintronics applications. Fe_3GeTe_2 is a van der Waals ferromagnet that is particularly promising for its high and electrically tunable curie temperature. We have recently observed using ARPES that both local magnetic moments and itinerant spin excitations play a cruicial role in describing the electronic ground state and the lowest energy excitations. In this work we performed first principle DFT calculations to verify our experimental discovery, with a special attention to creating a pipeline between the DFT results and the observed ARPES signal. This is enabled by wannierization of the DFT states, followed by the construction of a tight-binding model. We demonstrate that, including spin orbit coupling, our DFT bands show good agreement with the experimental ARPES bands.The further use of chinook [Day, R.P.,et al. npj Quantum Mater. 4, 54 (2019)] allows to compare calculations and experiments in the photoemission signal.

O 29.22 Tue 12:30 Poster A

Linear and circular dichroism ARPES of the charge density wave material $TiSe_2$ — •Hibiki Orio[1], Maximilian Ünzelmann[1], Jakub Schusser[1], Kai Rossnagel[2,3], and Friedrich Reinert[1] — [1]Universität Würzburg, Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence, Würzburg, Germany — [2]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [3]IEAP and KiNSIS, CAU Kiel, Kiel, Germany

The transition metal dichalcogenide compound $TiSe_2$ transforms into a $2 \times 2 \times 2$ charge density wave (CDW) phase below 200K. The physical process governing the buildup of the CDW has been controversial. To understand the nature of this intriguing property, the hybridized orbital character involved in the CDW gap formation is crucial information. Recent studies show that linear- and circular dichroism (LD and CD) in angle-resolved photoelectron spectroscopy (ARPES) provides insights into the orbital texture of the initial states. Here, using ARPES in the soft x-ray photon energy range, we systematically study the LD and CD of $TiSe_2$ in both the semimetallic and CDW phases.

O 29.23 Tue 12:30 Poster A

Spin polarisation of an Anderson impurity state in MoS2 mirror twin boundaries — •Tfyeche Y. Tounsi[1], Mahasweta Bagchi[1], Affan Safeer[1], Camiel van Efferen[1], Thomas Michely[1], Wouter Jolie[1], Theo A. Costi[2], and Jeison Fischer[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

Mirror twin boundaries (MTB) are line defects found in monolayer MoS2 islands grown via molecular beam epitaxy on graphene on Ir(111). MTBs form a well-defined 1D system of finite length, hosting confined states. When the highest occupied confined state is at the Fermi level, it splits into a singly occupied and doubly unoccupied states, defining an Anderson impurity. The interaction with the substrate electron bath establishes a Kondo resonance [1].

Here, spin-polarised scanning tunnelling spectroscopy measurements on an MTB in presence of out-of-plane magnetic field at a temperature of 0.4 K show an intensity change of the impurity peaks and Kondo resonance as a function of magnetic field. The experimental data is compared to numerical renormalization group calculations, demonstrating the full spin polarisation of both Anderson impurity sates and Kondo resonance.

[1] van Efferen et al., Nat. Phys. (2023).
https://doi.org/10.1038/s41567-023-02250-w.

O 29.24 Tue 12:30 Poster A

Optical characterization of sulfur vacancies in TMDCs under high vacuum — •Joel Verlande, André Maas, Leon Daniel, Lars Breuer, and Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik and CENIDE, Germany

The characterization of 2D Materials under non-ambient conditions offers the potential for a deeper analysis of various defects in the crystalline structure and their effects on the optoelectronic properties. Especially the investigation under a vacuum can provide us with crucial information about the actual influence of vacancies due to often occurring defect saturation by adsorbates, such as O_2 or N_2. These gas molecules can act as electron donors in the 2D structure that support the creation of negatively charged trions which have a higher rate of non radiating recombination. This results in a lower photoluminescent yield which could be an unfavourable property of the material.

For this study we generated sulfur vacancies in WS_2 and MoS_2 CVD-grown monolayers by irradiation with low energy Ar^+ ions ($E_{\mathrm{kin}} \leq 500$ eV). Subsequently the samples were analyzed by Raman and photoluminescence spectroscopy in a vacuum cell with pressures of $p < 10^{-4}$ mbar. The high vacuum leads to a dissipation of the gas molecules whereby we were able to examine the influence of the adsorbates on the weight of trionic and excitonic photoluminescent emission.

O 29.25 Tue 12:30 Poster A

Azimuthal- and valley dependent second harmonic generation response of monolayer MoS2 — •Jin Yu, Tao Yang, R. Kramer Campen, and YuJin Tong — Universität Duisburg-Essen, Fakultät für Physik, Experimentalphysik, Lotharstr. 1, 47057 Duisburg

Transition metal dichalcogenides (TMDCs) offer advantages in terms of rapid information processing speed and low energy consumption compared to conventional electronic components. Understanding how spin-valley locking controls the interaction of TMDCs and light is crucial for optimizing TMDCs for practical applications in quantum technology. In this study, we employed elliptically and circularly polarized lasers to excite monolayers of molybdenum disulfide. Our results reveal significant changes in the disappearance of sixfold symmetry, larger azimuthally dependent second harmonic generation (SHG) intensity extremes, and the rotation of a sixfold pattern due to variations in laser polarization from linear to circular and our data aligns closely with the predictions of the steady-state model. According to the steady-state model, under low-light-intensity excitation conditions, the angle of the sixfold pattern rotation is proportional to the difference in the number of particles between the valleys. This result provides a quantitative understanding of the SHG valley polarization signal.

O 29.26 Tue 12:30 Poster A

Integrated Computational Approach for the Treatment of 2D Heterostructures — •Anastasiia Nihei[1,2], Roman Kempt[1], Tom Barnowsky[1,2], Thomas Heine[1,2], Stefano Curtarolo[3], and Rico

Friedrich[1,2,3] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [3]Duke University, Durham, USA

Heterostructure interfaces of two-dimensional (2D) materials enable the realization of advanced electronic functionalities at the nanoscale. The efficient computational *ab initio* modelling of these systems is, however, a challenge as it requires the proper lattice matching of the component 2D sheets with minimal strain. This often results in large structures with hundreds to thousands of atoms.

Here, we utilize the newly developed hetbuilder tool to automate the heterotructure cell construction based on coincidence lattice theory [1,2]. It is integrated with the AFLOW materials database and software [3,4] allowing for an efficient workflow for the structure generation from the bulk parent systems. We benchmark the approach by performing *ab initio* calculations on several different heterostructures of 2D materials and study their electronic properties.

[1] D. S. Koda *et al.*, J. Phys. Chem. C **120**, 10895 (2016).
[2] https://zenodo.org/record/4721346.
[3] M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023).
[4] C. Oses *et al.*, Comput. Mater. Sci. **217**, 111889 (2023).

O 29.27 Tue 12:30 Poster A

Self-assembled Moiré superstructure of MXene — •Andrea Cabero del Hierro[1], Kuanysh Zhussupbekov[1,2], Samuel Berman[1], Dahnan Spurling[2], Ainur Zhussupbekova[1,2], David D. O'Regan[1], Igor V. Shvets[1], and Valeria Nicolosi[2,3] — [1]School of Physics, Trinity College Dublin, Dublin 2, D02 PN40, Ireland — [2]School of Chemistry, Trinity College Dublin, Dublin 2, D02 PN40, Ireland — [3]Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN) and Advanced Materials and Bioengineering Research (AMBER), Trinity College Dublin, Dublin 2, Ireland

The atomically reconstructed moiré superlattice and its impact on the microscopic electronic structure remains absent. In this investigation, we meticulously inspect and compare the self-assembled moiré superlattices of MXene. Employing a combination of experimental scanning tunneling microscopy/spectroscopy observations and ab initio simulations, we investigated three distinct self-assembled moiré patterns characterized by wavelengths approximately around 2.32 nm, 2.17 nm, and 1.12 nm. Our results illuminate a non-monotonic behavior in the moiré potential concerning periods on the valence band side. This research not only contributes to a detailed comprehension of MXene's moiré phenomena but also establishes a fresh foundation for further exploration into unique correlated phases.

O 29.28 Tue 12:30 Poster A

Exploring the structure of extended defects in MoS_2 bilayers with a machine-learned ACE potential — •Kevin Dhamo and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

Layered transition metal dichalcogenides (TMDs), for example MoS_2, have gathered much attention due to their unique tunable electrical, optical, thermal, and tribological properties. TMDs are usually applied as stacks of layers, which are prone to include extended defects such as in-plane dislocations or misalignments due to the rotation of subsequent layers. Density-functional theory (DFT) would be the method of choice to study the properties of such extended defects. However, the representation of extended defects often requires very large unit cells, which makes DFT calculations unfeasible.

In this work, we use DFT data to train an atomic cluster expansion (ACE) machine-learned interatomic potential for MoS_2. The capabilities of the ACE potential are benchmarked against DFT calculations of MoS_2 bilayers by comparing binding energy curves and Gamma surfaces for different bilayer stackings. Finally, the ACE potential is applied to study the structural properties of dislocations in MoS_2 bilayers and the atomic relaxations in the moiré pattern of twisted bilayer MoS_2 for different rotation angles.

O 29.29 Tue 12:30 Poster A

SNOM of lateral TMDC heterostructures — •Philipp Schwendke[1], Samuel Palato[1], and Julia Stähler[1,2] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der MPG

Semiconductor heterojunctions are the basis of many modern devices such as transistors, LEDs, and photovoltaics. 2D semiconductors such as TMDCs promise similar applications at an atomic level, which is why their interfaces are of particular interest. A variety of useful heterojunction properties have been realized, such as the photovoltaic effect and current rectification. While stacked van der Waals heterostructures ideally offer spatially homogeneous properties, lateral heterojunctions feature a lateral charge transfer following the band alignment across an interface region. Here, the charge carrier energy levels and lifetimes vary spatially in a way that is to date not fully understood. To explore said properties, we use scanning near-field optical microscopy (SNOM) combined with a femtosecond laser to investigate electron dynamics at ultrafast time scales with nm spatial resolution. Using previously introduced quadrature-assisted discrete (QUAD) demodulation, we are able to perform SNOM with a low repetition rate laser producing highly tunable fs laser pulses. QUAD demodulation is compatible with known methods of noise reduction, e.g. pseudo-heterodyne or balanced detection, and straightforward to extend into a pump-probe scheme for time resolution. This makes time-resolved SNOM an ideal candidate for the investigation of electronic properties of lateral heterojunctions.

O 29.30 Tue 12:30 Poster A

Compressed charges and interface dipoles persist at two-dimensional van der Waals heterojunctions — •Jae-Hyeok Ko[1], Giyeok Lee[1,3], Woosun Jang[2], and Aloysius Soon[1,3] — [1]Department of Materials Science & Engineering, Yonsei University, Seoul, Republic of Korea — [2]Integrated Science & Engineering Division, Underwood International College, Yonsei University, Incheon 21983, Republic of Korea — [3]School of Physics, University of Sydney, Sydney 2006, NSW, Australia

Heterojunctions of two-dimensional (2D) van der Waals (vdW) nanomaterials often exhibit unusual, "non-textbook" bonding mechanism that involves distinct orbital coupling within the compressed vdW gap. To unravel this atypical bonding mechanism for 2D heterointerfaces, using density-functional theory calculations, we examine the compressed charge redistribution and interface dipoles for the heterostructures of $ReSe_2$/graphene, $ReSe_2$/*h*-BN, and $ReSe_2$/*h*-BN/graphene. Here, we report the optimized atomic structures, electronic density-of-states, (integrated) planar-averaged electron density differences for these heterostructures, while focusing on the explicit contributions of the conductive graphene and insulating *h*-BN substrates to the interlayer confined charges and dipoles. Using other 2D heterosystems, we demonstrate that this charge compression effect in the vdW gap is ubiquitous and general regardless of the nature of the substrates and supports. This study highlights the importance of understanding the interlayer charges and dipoles and how this may contribute to the better designs of remote charge transfer systems in modern electronics.

O 29.31 Tue 12:30 Poster A

Unveiling the nature of atomic defects in graphene on a metal surface — •Karl Rothe, Nicolas Néel, and Jörg Kröger — TU Ilmenau, Institut für Physik

Argon ion bombardment of graphene-covered Ir(111) induces two types of atomic-scale defects. Using a scanning tunneling microscope, both defects appear as a depression without discernible interior structure suggesting the presence of vacancy sites in the graphene lattice. With an atomic force microscope, however, only one kind of defect can be identified as a site with missing carbon atoms, while the other kind reveals an intact graphene sheet. Spatially resolved spectroscopy of the differential conductance and the measurement of short-range force variations as a function of the lateral and vertical probe-defect distance corroborate the different character of the defects. The tendency of the vacancy defect to form a chemical bond with the microscope probe is reflected by the strongest attraction at the vacancy center as well as by hysteresis effects in force traces recorded for tip approach to and retraction from the Pauli repulsion range of vertical distances.

Financial support by the Deutsche Forschungsgemeinschaft through Grant No. KR 2912/17-1 is acknowledged.

O 29.32 Tue 12:30 Poster A

Characterising nitrogen defects in graphene grown by bottom-up synthesis — •Liv Warwick[1,2], Matthew A. Stoodley[2,3], Jonathan Bradford[1], Matthew Edmondson[1], Benedikt P. Klein[2,3], Fulden Eratam[2], Henry P. Hoddinott[2,4], Luke A. Rochford[5], Reinhard J. Maurer[3], David A. Duncan[2], and Alex Saywell[1] — [1]University of Nottingham, Nottingham, UK — [2]Diamond Light Source, Didcot, UK — [3]University of Warwick, Coventry, UK — [4]University of Swansea, Swansea, UK — [5]University of Cambridge, Cambridge, UK

Recently, we have pioneered a new method for the growth of defective graphene, e.g. graphitic material containing heteroatoms or vacancies, [1] by 'bottom-up' on-surface growth methodologies. In our chemical vapour deposition process [2] we use an aromatic precursor that contains the same structural element as our desired defects. Here, using a similar method, we will present a low temperature scanning tunnelling microscopy (LT-STM), X-ray photoelectron spectroscopy (XPS) and normal incidence X-ray standing waves (NIXSW) study of graphene containing nitrogen defects, grown from a nitrogen containing precursor. By transferring the samples between the different technique chambers via an ultra-high vacuum suitcase, we were able to correlate spectroscopic differences to morphological changes on the surface.

[1] Bhatt, M. D. et al. RSC Adv. 12, 21520-21547 (2022) [2] B. P. Klein. et al. Appl. Phys. Lett., 2022, 121, 191603.

O 29.33 Tue 12:30 Poster A

Intermediate diffusive-ballistic electron conduction around mesoscopic defects in graphene layers — Toni Marković[1], Wei Huang[1], William S. Huxter[2], Pietro Gambardella[1], and •Sebastian Stepanow[1] — [1]Department of Materials, ETH Zurich — [2]Department of Physics, ETH Zurich

Non-diffusive effects in charge transport become relevant as device sizes and features become comparable to the electronic mean free path. As a model system, we investigate the spatial transport around mesoscopic defects, which we refer to as pits, in graphene with scanning tunneling potentiometry. Diffusive and ballistic contributions to the transport dipole are investigated by simultaneously resolving the nanoscale topography of the pits and measuring the local electrochemical potential change in the surrounding area. We find evidence of transport in the intermediate regime between diffusive and ballistic limits, as the potential changes around pits are substantially underestimated by diffusive models. We also observe a dependence of the dipole magnitude on the shape of the pits. Our experiments and modelling are supported by lattice Boltzmann simulations, which highlights the importance of the ratio between the pit size and the mean free path in the intermediate transport regime.

O 29.34 Tue 12:30 Poster A

Imaging the local Electrochemical Potential of Graphene with Scanning Tunneling Potentiometry — Toni Marković, Wei Huang, •Mark Canavan, Jeong Ah Seo, Pietro Gambardella, and Sebastian Stepanow — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Two-dimensional material systems and heterostructures have recently emerged as a promising class of materials for high performance electronic devices. In such systems, understanding the influence nanoscale transport effects, such as scattering at atomic defects and interfaces is crucial. Scanning Tunneling Potentiometry (STP) allows for studying charge transport on the nanoscale by relating the local electro-chemical potential to morphological features of the system. STP maintains the angstrom spatial sensitivity of conventional STM while imaging modifications to the ECP with uV resolution, offering a way to potentially investigate transport phenomena beyond the diffusive regime. Here, we present an implementation of STP in a commercial RHK Pan-Scan STM with an integrated flow cryostat capable of reaching temperatures of 12K [1]. We perform STP on epitaxial graphene to measure the sheet resistance of monolayer and bilayer grown on SiC as well resistances of interfaces between them. To investigate transport effects beyond the diffusive regime, using back-gated graphene samples would allow for STP measurements with charge carries at the Dirac point.

[1] T. Marković et al. Rev. Sci. Instrum. 92, 103707 (2021)

O 29.35 Tue 12:30 Poster A

Observation of different Li intercalation states and local doping in epitaxial mono- and bilayer graphene on SiC(0001) — Wei Huang, •Jeongah Seo, Mark Canavan, Pietro Gambardella, and Sebastian Stepanow — Department of Materials, ETH Zurich, Switzerland

Li intercalation is commonly used to enhance the carrier density in epitaxial graphene and mitigate coupling to the substrate. So far, the understanding of the intercalation process, particularly how Li penetrates different layers above the substrate, and its impact on electron transport remains incomplete. Here, we report different phases of Li intercalation and their kinetic processes in epitaxial mono- and bilayer graphene grown on SiC. The distinct doping effects of each intercalation phase are characterized using scanning tunneling spectroscopy. Furthermore, changes in the local conduction regimes are directly mapped by scanning tunneling potentiometry and attributed to different charge transfer states of the intercalated Li. The stable intercalation marked by the formation of Li-Si bonds leads to significant 56% reduction in sheet resistance of the resulting quasi-free bilayer graphene, as compared to the pristine monolayer graphene.