

O 79: 2D Materials V: Growth, Structure and Substrate Interaction

Time: Thursday 10:30–13:00

Location: MA 005

O 79.1 Thu 10:30 MA 005

Exfoliation of large-area monolayers using template stripped gold — ●LAXMAN NAGIREDDY^{1,2,3}, NEIL R. WILSON¹, MARIA CHRISTINE RICHTER^{2,3}, KAROL HRICOVINI^{2,3}, MATTHEW D. WATSON⁴, CEPHISE CACHO⁴, NICHOLAS D. M. HINE¹, and SAMUEL J. MAGORRIAN¹ — ¹University of Warwick, Coventry, UK — ²CY Cergy Paris Université, CEA, LIDYL, Gif-sur-Yvette, France — ³Université Paris-Saclay, CEA, LIDYL, Gif-sur-Yvette, France — ⁴Diamond Light Source, Harwell Science and Innovation Campus, Didcot, UK

The diverse family of two-dimensional materials exhibits a myriad of applications owing to their unique electronic, optical, and chemical properties. While mechanical exfoliation has been a pivotal method for obtaining high-quality two-dimensional materials, existing techniques are constrained by limitations in yield, lateral size, and contamination. Although numerous studies have explored the use of gold for exfoliating large-area monolayers [1], these approaches often prove unsuitable for surface-sensitive techniques such as photoemission spectroscopy.

In this study, we present a novel methodology for preparing an atomically flat gold surface using a template stripped gold method [2], subsequently employed for the exfoliation of various two-dimensional materials. Successful exfoliation was achieved for WSe₂, CrSBr, and FePS₃. The obtained monolayers were characterized using angle-resolved photoemission spectroscopy (ARPES).

References:

- [1] M Velicky, et al., ACSnano 12.10 10463-10472 (2018).
- [2] N Vogel, et al., Nanoscale 4.13 3820-3832 (2012).

O 79.2 Thu 10:45 MA 005

Janus SeMoS monolayers grown by chemical vapor deposition on Au(111) — ●JULIAN PICKER¹, MAHDI GHOORBANI-ASL², MAXIMILIAN SCHAAL³, SILVAN KRETSCHMER², FELIX OTTO³, MARCO GRUENEWALD³, CHRISTOF NEUMANN¹, ANTONY GEORGE¹, TORSTEN FRITZ³, ARKADY KRASHENINNIKOV², and ANDREY TURCHANIN¹ — ¹Institute of Physical Chemistry, Friedrich Schiller University Jena — ²Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf — ³Institute of Solid State Physics, Friedrich Schiller University Jena

Janus transition metal dichalcogenide monolayers (TMD MLs) are asymmetric two-dimensional (2D) crystals consisting of two different chalcogens on their opposite faces. Their unique structure results in the in-built electric dipole and leads to new physical phenomena compared to conventional TMD MLs such as MoS₂ or MoSe₂. Here we report an epitaxial growth of Janus SeMoS MLs on Au(111) by chemical vapor deposition. In the growth process, sulfur atoms intercalate between the MoSe₂ ML and Au(111) resulting in the exchange of the bottom selenium layer with sulfur [1]. We studied the structure of the formed Janus SeMoS MLs by scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). The electronic structure was characterized by angle-resolved photoelectron spectroscopy (ARPES). Density functional theory (DFT) calculations demonstrate a good agreement with the experimental findings.

- [1] Z. Gan *et al.*, Adv. Mater. **34**, 2205226 (2022).

O 79.3 Thu 11:00 MA 005

Growth of Titanium Ditelluride on Au(111) — ●ANDREAS RAABGRUND, HANNAH LOH, ALEXANDER WEGERICH, TILMAN KISSLINGER, LUTZ HAMMER, and M. ALEXANDER SCHNEIDER — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Aiming at the MBE growth of transition metal ditelluride (MTe₂) films, especially in the monolayer limit, the formation of and interaction with the substrate interface is of fundamental interest. The growth of a MTe₂ film can be achieved either by the tellurization of the desired metal substrate [1] or by the deposition of Te [2] or any other chalcogenide [3] and a desired transition metal on a substrate of suitable choice.

In this contribution we follow the latter approach and investigate tellurium and titanium on Au(111) by LEED-IV, DFT, and STM. Starting from submonolayer coverages of Ti and Te, a first stable, ordered (3√3 × 3√3)R30° superstructure is found. With increasing amount of Ti and a proper annealing step a (5 × √3)_{rect} structure develops. For higher amounts of Te and Ti, a closed hexagonal film with a lateral lattice parameter of 4/3 times that of Au(111) is found by LEED and

STM. STM topography and spectroscopy measurements indicate the growth of a TiTe₂ layer on a Te containing interface to the Au(111) substrate.

- [1] T. Kiklinger *et al.*, Phys. Rev. B **108**, 205412 (2023)
- [2] K. Lasek *et al.*, ACS Nano **14**, 8473 (2020)
- [3] S. G. Sørensen *et al.*, ACS Nano **8**, 6788 (2014)

O 79.4 Thu 11:15 MA 005

Influence of the substrate on pore creation in single-layer MoS₂ using highly charged ion irradiation — ●YOSSARIAN LIEBSCH¹, LEON DANIEL¹, LUCIA SKOPINSKI¹, CAROLIN FRANK¹, UMAIR JAVED², JANI KOTAKOSKI², and MARIKA SCHLEBERGER² — ¹University Duisburg-Essen, Duisburg, Germany — ²Universität Wien, Vienna, Austria

Ion irradiation serves as a versatile tool for modifying 2D materials and surfaces, enabling the creation of defects, pores, and incisions. However, characterizing the nanometer-sized structural changes induced by ion irradiation has proven challenging, often necessitating high-resolution TEM. Notably, direct characterization of such defects has primarily focused on suspended 2D materials, neglecting the substrate's influence on defect formation during irradiation. To address this issue, we irradiated single-layer MoS₂ on a Si/SiO₂ substrate using highly charged ions (HCIs) at 20 keV and 180 keV and different charge states. Subsequently, the material was transferred to a TEM-grid and analyzed using scanning transmission electron microscopy (STEM). Well-defined, round pores were observed for all kinetic and potential energies, indicating a rather small influence of sputtered substrate material. In contrast to suspended MoS₂, significant differences in both pore size and creation efficiency were evident. These observations hold particular significance for 2D material applications that utilize ion irradiation as a mean to create pores and catalytically active sites, as they allow for a precise control of pore density and defective area by choosing appropriate irradiation parameters.

O 79.5 Thu 11:30 MA 005

Phase engineering in tantalum sulfide monolayers on Au(111) — DANIELA DOMBROWSKI^{1,2}, ABDUS SAMAD³, KAI MEHLICH¹, UDO SCHWINGENSCHLÖGL³, ●THAIS CHAGAS¹, and CARSTEN BUSSE^{1,2} — ¹Department Physik, Universität Siegen, Germany — ²Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — ³Physical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Saudi Arabia

We prepare monolayers of tantalum sulfide on Au(111) by evaporation of Ta in a reactive background of H₂S. Under sulfur-rich conditions, monolayers of 2H-TaS₂ develop, whereas under sulfur-poor conditions TaS forms, a structure that can be derived from 2H-TaS₂ by removal of the bottom S layer. We analyze the alignment of the layers with respect to the substrate and the relation with the domains in the Au(111) herringbone reconstruction using scanning tunneling microscopy. With the help of density functional theory calculations, we can determine the registry of the two phases with the substrate. We develop a growth process that allows the preparation of uniquely oriented 2H-TaS₂ on Au(111). 2H-TaS₂ and TaS have a remarkably similar in-plane lattice structure and we observe the formation of lateral 2H-TaS₂-TaS heterostructures with atomically well-defined and defect-free boundaries. We observe mirror twin boundaries within 2H-TaS₂ along the S- and Ta-edge.

O 79.6 Thu 11:45 MA 005

Isolating the optical response of a MoS₂ monolayer under extreme screening of a metal — ●TAO YANG¹, STEPHAN SLEZIONA¹, ERIK POLLMANN¹, ECKART HASSELBRINK², PETER KRATZER¹, MARIKA SCHLEBERGER¹, R. KRAMER CAMPEN¹, and YUJIN TONG¹ — ¹Fakultät für Physik, Universität of Duisburg-Essen, Germany — ²Fakultät für Chemie, Universität of Duisburg-Essen, Germany

Transition metal dichalcogenides monolayers, as two-dimensional (2D) direct bandgap semiconductors, hold promise for advanced optoelectronic and photocatalytic devices. Interaction with three-dimensional (3D) metals, like Au, profoundly affects their optical properties, posing challenges in characterizing the monolayer's optical responses within the semiconductor-metal junction. In this study, using pre-

cise polarization-controlled final-state sum frequency generation (FS-SFG), we successfully isolated the optical responses of a MoS₂ monolayer from a MoS₂/Au junction. The resulting SFG spectra exhibit a linear lineshape without A or B exciton features, attributed to strong dielectric screening and substrate induced doping. The linear lineshape illustrates the expected constant density of states at the band edge of the 2D semiconductor, typically obscured by excitonic interactions in weak-screening conditions. Extrapolation yields the onset of a direct quasiparticle bandgap of about 1.65 ± 0.20 eV, indicating significant bandgap renormalization. This study enriches understanding of the optical responses of a 2D semiconductor in extreme screening conditions and provides a critical reference for 2D semiconductor-based photocatalytic applications.

O 79.7 Thu 12:00 MA 005

Direct Beam-Induced Chemical Etching of 2D Materials in Transmission Electron Microscope — •MITISHA JAIN, SILVAN KRETSCHMER, and ARKADY KRASHENINNIKOV — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

The interaction of energetic electrons with the specimen during imaging in a transmission electron microscope (TEM) can give rise to the formation of defects or even complete destruction of the sample. This is particularly relevant to atomically thin two-dimensional (2D) materials. Depending on electron energy and material type, different mechanisms such as knock-on (ballistic) damage, inelastic interactions including ionization and excitations, as well as beam-mediated chemical etching can govern defect production. Using first-principles calculations combined with the McKinley-Feshbach formalism, we investigate the latter channel of damage creation in two representative 2D materials, MoS₂ and h-BN with adsorbed single adatoms (H, C, N, O, etc.), which can originate from molecules always present in the TEM column. We assess the ballistic displacement threshold energies T for the host atoms in 2D materials when adatoms are present and demonstrate that T can be reduced, as chemical bonds are locally weakened due to the formation of new bonds with the adatom. We conclude that while adatoms should play a role in damage creation in MoS₂, formation of defects in h-BN sheets at electron energies well below the knock-on threshold cannot be explained by the presence of adatoms, that is by the direct electron beam-induced chemical etching.

O 79.8 Thu 12:15 MA 005

Optoelectronic Interactions of WS₂-ZnO for Scalable LEDs Based on Two-Dimensional Materials — •OSAMAH KHARSAH¹, LEON DANIEL¹, DENYS VIDISH², DEDI SUTARMA¹, JONAH VON KUCZKOWSKI¹, STEPHAN SLEZIONA¹, ULRICH HAGEMANN³, KEVIN MUSSELMAN², and MARIKA SCHLEBERGER¹ — ¹Universität Duisburg-Essen, Fakultät für Physik and CENIDE, Duisburg, Germany — ²University of Waterloo, Mechanical and Mechatronics Engineering, Waterloo, Canada — ³Interdisciplinary Center for Analytics on the Nanoscale (ICAN) and CENIDE, Duisburg, Germany

Two-dimensional tungsten disulfide (WS₂) is a promising material for scalable large-area light-emitting diodes (LED) due to its direct bandgap, stability, and high photoluminescence (PL). Teamed with zinc oxide (ZnO), an electron-transport n-type semiconductor, they form the basis for an n-i-p LED architecture. This study explores the interactions between WS₂ and both single-crystalline ZnO and spatial atomic layer deposition (SALD)-grown ZnO. Emphasizing the opto-

electronic interaction of this heterostructure, various characterization techniques such as PL and Raman spectroscopy, Atomic Force Microscopy, Kelvin Probe Force Microscopy, and X-ray Photoelectron Spectroscopy are employed. The results reveal a stronger optoelectronic interaction in WS₂-SALD ZnO, attributed to higher strain. Furthermore, we observe energy-level alignment at the interface in both cases, while noting the presence of OH groups in SALD ZnO but their absence in single-crystalline ZnO.

O 79.9 Thu 12:30 MA 005

Atomically thin transition metal halide NiBr₂ grown on Au(111) — •DANIEL ROTHHARDT^{1,2,3}, ZUNED AHMEND^{1,2}, CHRISTOPHER PENSCHKE⁴, HAO LIU^{1,2}, REGINA HOFFMANN-VOGEL³, PETER SAALFRANK⁴, HANS JOSEF HUG^{1,2}, and AMINA KIMOUCHE³ — ¹Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland — ²Department of Physics, University of Basel, CH-4056 Basel, Switzerland — ³Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany — ⁴Institute of Chemistry, University of Potsdam, 14476 Potsdam-Golm, Germany

In recent years, two-dimensional (2D) van der Waals materials have emerged as a new platform for studying low-dimensional quantum phenomena. Due to their limited symmetry, they display electrical, optical, and magnetic properties that are different compared to their 3D counterparts. As novel 2D materials, transition metal dihalides (TMHs) emerge as promising platform for stable ferro- or antiferromagnetic ordering in two dimensions. Epitaxial single-layer TMHs require accurate control of the growth parameters and an improved understanding of the interactions between TMHs and the surface. In this work, we employ frequency-modulated scanning force microscopy in the non-contact mode, combined with Kelvin probe microscopy and scanning tunneling microscopy, to examine various phases and layer thicknesses of NiBr₂ on Au(111) revealing a complicated growth mode in the low coverage regime.

O 79.10 Thu 12:45 MA 005

Atomically precise vacancy lattices in epitaxially grown FeBr₂ and CoBr₂ on Au(111) — FEIFEI XIANG¹, NEETA BISHT², BINBIN DA¹, CHRISTIAN NEISS², ANDREAS GÖRLING², and •SABINE MAIER¹ — ¹Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — ²Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

The generation of extensive 2D periodic patterns of point defects in 2D materials, such as vacancy lattices, has been a challenging task until now. We report on the growth and structure of epitaxially grown 2D transition metal dihalides on Au(111) featuring periodically assembled halogen vacancies that result in alternating coordination of the transition metal ion and can function as antidot lattices.[1] Using low-temperature STM/ncAFM and LEED, we identified the structural properties of intrinsically patterned FeBr₂ and CoBr₂ monolayers grown epitaxially on Au(111). Density-functional theory indicates that Br-vacancies are favored due to low formation energies, and the formation of a vacancy lattice substantially reduces the lattice mismatch with the underlying Au(111). We demonstrate that interfacial strain engineering presents a versatile strategy for controlled patterning in 2D with atomic precision over several hundred nanometers to solve a longstanding challenge of growing atomically precise antidot lattices. [1] F. Xiang, et al. arXiv preprint arXiv:2305.06489, 2023.