TT 16: 2D Materials beyond graphene: Growth, structure and substrate interaction (joint session O/HL/TT)

Time: Monday 15:00–17:45 Location: HSZ/0204

TT 16.1 Mon 15:00 HSZ/0204

A virtual super-moiré: $MnBr_2$ on graphene on Ir(110) — Affan Safeer[1], Oktay Güleryüz[1], Nicolae Atodiresei[2], •Thomas Michely[1], and Jeison Fischer[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

$MnBr_2$ on Gr/Ir(110) constitutes a three lattice system, giving rise to a super-moiré pattern – a moiré of moirés. The super-moiré of $Gr/MnBr_2/Ir(110)$ is unique, as it involves a virtual moiré of $MnBr_2$ with the Ir(110) surface lattice – two lattices not in contact with each other. Using a careful Fourier analysis of the bias dependence of scanning tunneling microscope topographs, scanning tunneling spectroscopy, the known properties of Gr/Ir(110), and the results of ab initio calculations, the origin of the virtual moiré is uncovered and related to the inhomogeneous binding of Gr to Ir(110). Comparative experiments with $MnBr_2$ on Gr/Ir(111) show similar growth and structure as on Gr/Ir(110), but highlight the unique properties of the $MnBr_2/Gr/Ir(110)$ super-moiré.

TT 16.2 Mon 15:15 HSZ/0204

Magnetism of monolayers of $FeCl_2$ and $FeBr_2$ Epitaxially Grown on Bi_2Se_3 — •Sebastien E. Hadjadj[1], Weibin Li[2], Pierluigi Gargiani[2], Cinthia Piamonteze[3], Oleksandr Stetsovych[4], Pavel Jelínek[4], Maxim Ilyn[1], and Celia Rogero[1] — [1]Materials Physics Center(MPC - CFM), Donostia, Spain — [2]ALBA Synchrotron Light Source, Barcelona, Spain — [3]Paul Scherrer Institut, Villigen, Switzerland — [4]FZU - Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

Two-dimensional transition metal dihalides exhibit novel magnetic and electronic properties. By combining 2D magnetic semiconductors with topological insulators (TIs) novel quantum and spintronic phenomena can be investigated. Here, we report the uniform and epitaxial growth of monolayer $FeCl_2$ and $FeBr_2$ on the TI Bi_2Se_3. Structural and electronic characterization via LEED, STM, and STS measurements revealed a material-specific moiré pattern resulting from lattice mismatch, as well as a position-independent bandgap of 4 eV. Synchrotron-radiation-based XAS and XMCD measurements confirm robust ferromagnetic order down to the monolayer limit, with an intrinsic reduction of the effective spin magnetic moment by 40-50%. These magnetic vdW heterostructures provide a platform for investigating magnetic proximity effects and moiré-induced modifications of topological surface states. [1] S. E. Hadjadj et al., Chem. Mater., 35, 23, 9847*9856,(2023) [2] S. Kerschbaumer et al., Adv. Science, e08262,(2025)

TT 16.3 Mon 15:30 HSZ/0204

Rise and fall of 1T-TaS_2: Epitaxial growth of monolayer TaS_2 on Au(111) — •Lars Buss[1], Cathy Sulaiman[1], Raquel Sánchez-Barquilla[1], Iulia Cojocariu[2], Marcin Szpytma[3], Tevfik Onur Menteş[2], Andrea Locatelli[2], Jens Falta[4], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Elettra-Sincrotrone Trieste S.C.p.A, Basovizza, Trieste, Italy — [3]Faculty of Physics and Applied Computer Science, AGH University of Krakow, Poland — [4]Institute of Solid State Physics, University of Bremen, Germany

Two-dimensional TaS_2 has attracted extensive research interest due to its ability to exhibit electron correlation effects, including charge density waves (CDWs). In particular, 1T-TaS_2 is of interest as it shows a CDW at room temperature. However, when grown on metal substrates, only 2H-TaS_2 has been reported. To elucidate the reasons for the apparent lack of 1T-TaS_2 growth in the literature, we have investigated the growth of TaS_2 on Au(111) employing *in situ* low-energy electron microscopy (LEEM) and micro-diffraction (μLEED) as well as X-ray photoemission electron microscopy (XPEEM) [1]. We show that at elevated temperatures TaS_2 nucleates and grows in the metastable 1T-TaS_2 phase, which transforms into the stable 2H-TaS_2 phase via a temperature-activated process and then continues to grow at a considerably lower rate. Furthermore, we observe CDW-like ordering in 1T-TaS_2/Au(111), though it is suppressed in 2H-TaS_2/Au(111).

[1] L. Buß et al. Phys. Rev. Materials **9**, 074006 (2025).

TT 16.4 Mon 15:45 HSZ/0204

Band-Like Transport and its Modulation by Nitrogen Doping in Transferable Semi-Conducting 2D-imine Covalent Organic Framework — •Vijay Bahadur Yadav, Diksha Srivastava, Satya Veer Singh, Itu Pandey, Manabendra Chandra, and Thiruvancheril G. Gopakumar — Indian Institute of Technology Kanpur

Two-dimensional (2D) imine-based covalent organic frameworks (COFs) are promising semiconductors for thin-film electronics and sensing due to their extended in-plane π-conjugation, enabling efficient charge transport. Here, we investigate two highly crystalline 2D imine COF films synthesised via quasi-equilibrium Schiff base condensation. By selecting molecular precursors, we tuned the nitrogen content, producing COFs with ten and six nitrogen atoms per unit cell (10N-COF and 6N-COF). The films are chemically stable in organic solvents and water, mechanically robust, and transferable onto various substrates, allowing fabrication over areas of tens of square centimeters. Electrical measurements using silver electrode arrays show linear current*voltage behaviour, indicating band-like transport, with consistent responses across multiple regions. The conductivity of 10N-COF is ~36 times higher than that of 6N-COF. Density functional theory calculations reveal similar band gaps but enhanced band dispersion near the Fermi level in 10N-COF, improving charge carrier mobility. Nitrogen incorporation thus effectively tunes charge transport in 2D COFs.

TT 16.5 Mon 16:00 HSZ/0204

Co_2S_2: a new 2D material and its phase transitions — •Abdallah Karaka, Max Wolfertz, Affan Safeer, Guangyao Miao, Wouter Jolie, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

Using molecular beam epitaxy under ultra high vacuum conditions, 2D materials can be synthesized under conditions far from equilibrium for which no bulk parent compound exists.

Co_2S_2-2D is such an example. Using scanning tunneling microscopy and low energy electron diffraction we characterize this new single-layer 2D material crystallizing in the CuI structure (space group: $P\bar{3}m1$ trigonal), when grown on graphene on Ir(111) using molecular beam epitaxy. We found it can be synthesized phase pure upon low temperature growth and moderate annealing with a lattice constant of 3.66 ± 0.05 Å and a height of 6.2 Å. Beyond the single-layer limit it transforms into a new hexagonal crystal structure with a distinctly different lattice parameter of 3.52 ± 0.05 Å and a height of 11.7 Å. This transition typically occurs between 650 and 750 K, although the exact temperature depends on the annealing conditions. The phase transition is accompanied by the emergence of a 2x2 superstructure in the high temperature phase.

TT 16.6 Mon 16:15 HSZ/0204

Tailored growth of 2D alloy transition metal dichalcogenides with tunable optical and electrical properties using liquid precursors — •Md Tarik Hossain[1], Axel Printschler[1], Nhat Lam Duong[1], Julian Picker[1], Rahul Sharma[1], Christof Neumann[1], Mona Sedighi[2], Johannes Biskupek[2], Muhammad Sufyan Ramzan[1], Caterina Cocchi[1], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Jena, Germany — [2]University of Ulm, Ulm, Germany

Doping or alloying of two-dimensional (2D) transition metal dichalcogenides (TMDs) provides a promising route to tune the optical, magnetic, and electronic properties. Here, we present a liquid-precursor-based chemical vapor deposition (CVD) for the controlled growth of large-area monolayer $(V_xW_zMo_{1-x-y})S_2$ alloys with tunable optical and electrical properties. Comprehensive characterization using atomic force microscopy, transmission electron microscopy, Raman spectroscopy, photoluminescence (PL) spectroscopy, and ab initio calculations confirms the structural and optical quality. Notably, PL shows a noticeable defect exciton peak at room temperature in the V-doped monolayer. Furthermore, by adjusting the composition, we modulate the carrier type of these monolayers from n-type to p-type or even make the monolayers metallic for high vanadium concentrations, which is deduced from electrical transport measurements and density

functional theory calculations. This work demonstrates high potential of liquid-precursor CVD as a platform for the tailored growth of complex 2D TMD alloys for next-generation optoelectronic devices.

TT 16.7 Mon 16:30 HSZ/0204

CVD growth and characterization of WSe_2 monolayers on Au(111) and their conversion to Janus SeWS — •Julian Picker[1], Jonas Brandhoff[2], Maximilian Schaal[2], Felix Otto[2], Christof Neumann[1], Torsten Fritz[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Transition metal dichalcogenides (TMDs) exhibit distinctive optical and electronic properties in the two-dimensional monolayer limit. Recently, Janus TMDs have attracted significant attention because their asymmetric chalcogen composition breaks the out-of-plane symmetry and enables properties not attainable in conventional TMDs. In this work, we initially investigate the structural and electronic characteristics of WSe_2 monolayers grown on Au(111) via ambient-pressure chemical vapor deposition (CVD). Surface-sensitive techniques - including scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), and angle-resolved photoelectron spectroscopy (ARPES) - were employed to characterize the properties of these monolayers. Subsequently, the WSe_2 monolayers were transformed into Janus SeWS monolayers through selective chalcogen replacement at the WSe_2/Au interface. A comparative analysis reveals the structural and electronic differences between the two systems.

TT 16.8 Mon 16:45 HSZ/0204

Controlling polymorphism in the growth of 2D manganese sulfide on graphene via substrate interaction — •Max Wolfertz, Abdallah Karaka, Nicolas Georgopoulos, Oktay Güleryüz, Affan Safeer, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

We investigate the epitaxial growth of single-layer manganese sulfide on graphene/Ir substrates grown via molecular beam epitaxy. Morphology, crystal structure and electronic properties are examined using scanning tunneling microscopy and - spectroscopy and low energy electron diffraction. While bulk MnS exists in the three polymorphs, α-(rock-salt structure), β-(zincblende structure), and γ-MnS (wurtzite structure), its structure in a single-layer is unknown, as fabrication using exfoliation methods cannot be applied. We find that when grown by molecular beam epitaxy on Gr/Ir substrates manganese sulfide grows in two competing phases: manganese sulfide in trigonal CuI-structure (space group P-3m1) and MnS in thin platelets of a cubic rock-salt structure (space group Fm-3m). Their in-plane lattice parameters are 4.16 Å, and 3.63 Å respectively. We show that the substrate exerts a strong influence on the phase selected. While the growth on Gr/Ir(111) results in a large share of cubic MnS, the Gr/Ir(110) substrate favors the formation of single layer trigonal manganese sulfide. Also, the use of seeding methods for avoiding loss of Mn into the bulk Ir crystals is discussed.

TT 16.9 Mon 17:00 HSZ/0204

Low Temperature MOCVD Growth of two-dimensional InSe and InSe/WS2 Heterostructures — •Robin Guenkel, Nils Langlotz, Matvei Kislitsyn, Juergen Belz, and Kerstin Volz — mar.quest|Marburg Center for Quantum Materials and Sustainable Technologies, Philipps University Marburg, Germany

Two-dimensional van der Waals heterostructures offer powerful opportunities for engineered optoelectronic functionality, particularly when type-II band alignment enables efficient charge separation and interlayer transitions. InSe and WS* are especially promising in this regard because their band structures allow for the formation of a type-II interface at the Γ point, which avoids momentum mismatch. This is an essential requirement for robust radiative processes in 2D stacks. This talk presents a low-temperature metal-organic chemical vapor deposition (MOCVD) approach for synthesizing high-quality InSe and vertically integrated InSe/WS2 heterostructures. Using DTBSe and TMIn at 350 °C, we synthesize homogeneous, single-phase InSe films on 2-inch sapphire substrates and extend the process to directly grow on monolayer WS2. Atomic force microscopy, Raman spectroscopy, and energy-dispersive X-ray spectroscopy provide insight into the morphology, crystallinity, and composition of the films, offering a detailed understanding of the growth behavior and the influence of the substrate surface chemistry.

TT 16.10 Mon 17:15 HSZ/0204

Synthesis of Vertically Stacked 2D-hBN/Borophene Heterostructures on Ir(111) via Intrinsic Segregation — •Marko Kriegel, Karim Omambac, Smruti Mohanty, Birk Finke, Frank-J. Meyer zu Heringdorf, and Michael Horn-von Hoegen — University Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CENIDE), Lotharstr. 1, 47057 Duisburg, Germany

Research efforts on 2D materials increasingly target complex architectures built from high-quality heterostructures. A key challenge remains the reliable and scalable in-situ fabrication of such systems. In this work, we use high-resolution spot-profile analysis LEED (SPA-LEED) and -microscopy (LEEM) to investigate a synthesis route for an hBN/borophene heterostructure on Ir(111) based on *intrinsic segregation*. At elevated temperatures, boron dissolves into the Ir subsurface region during exposure to the borazine precursor $B_3N_3H_6$ in a CVD process [1], thereby creating a boron reservoir. Increasing the precursor pressure drives the chemical balance toward formation of a complete hBN layer across the Ir surface [2]. Upon cooldown, the decreasing boron solubility induces segregation, resulting in the growth of a continuous borophene layer beneath the hBN overlayer. This one-step CVD approach establishes a promising, scalable pathway for the controlled synthesis of high-quality 2D heterostructures. [1] K. Omambac et al., ACS Nano **15** (2021) 7421 [2] K. Omambac et al., ACS Nano **17** (2023) 17946

TT 16.11 Mon 17:30 HSZ/0204

MBE growth and characterization of high-quality monolayer MoS2 on stepped Au surface — •Sayan Debnath, Ram Prakash Pandeya, Konstantin Shchukin, Patrik Staudenmayer, and Alexander Grüneis — Optoelektronische Materialien Institut für Festkörperelektronik, TU Wien, 1040 Wien, Austria

In the present work, we investigate the growth of sub-monolayer MoS2 on Au(788) and Au(111), using molecular beam epitaxy. Sample growth quality is characterized using low-energy electron diffraction, X-ray photoemission spectroscopy, and scanning electron microscopy. Furthermore, a comparative study of the electronic properties was performed by studying the band structure using angle-resolved photoemission spectroscopy (ARPES), and the vibrational properties were measured by angle-resolved polarized Raman (ARPR) spectroscopy.

Our study reveals superior crystalline quality, with fewer S deficiencies, and better azimuthal order of MoS2 grown on the stepped Au(788) substrate compared to the Au(111). In the case of ARPES, we observed more resolved band dispersion on MoS2/Au (788), confirmed by probing the spin-orbit splitting at the Brillouin zone boundary (K point). On the other hand, ARPR of the first Raman mode E2g on MoS2/Au (788) deviates from the symmetry of freestanding MoS2, suggesting the effect of the stepped surface on the vibrational properties. We discuss the role of increased catalytic activity at step edges in promoting the growth of high-quality TMDCs, such as MoS2 and WS2, on stepped surfaces.