O 14: 2D Materials Beyond Graphene: Growth, Structure and Substrate Interaction (joint session O/HL)

Time: Monday 15:00–18:00 Location: H11

O 14.1 Mon 15:00 H11

Hexagonal structures of europium oxides on Pd(111) studied with LEED and STM — •Muriel Wegner, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Germany

With an increasing interest in technological applications of oxide materials, also two-dimensional (2D) oxides came into focus. The large flexibility in the variation of the cationic species, including even a combination of different cations, promises a rich variety of properties [1,2]. So far, the center of attention has been on transition metal sesquioxides M_2O_3 of corundum structure.

Here, we expand this field towards lanthanides. We present a combined scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) study of the growth of submonolayer coverages of europium oxide on a Pd(111) surface. Upon annealing the as deposited Eu in oxygen containing environments at temperatures above 800 K, long-range ordered multilayer islands of Eu_2O_3 are obtained. From LEED a $\begin{pmatrix} 8/3 & 4/3 \\ -4/3 & 4/3 \end{pmatrix}$ superstructure on Pd(111) is derived, which corresponds to a hexagonal lattice with a lattice parameter of 6.35 Å. This structure exhibits a large stability range. Only upon annealing to 1175 K in UHV an additional (2×2) superstructure evolves, which is seen as a hexagonal array of pores at a distance of 12.70 Å in STM. By addition of small amounts of Ti atoms, the transformation into planar two-dimensional films is achieved. These mixed-metal oxides form a honeycomb lattice with a lattice parameter of 7.2 Å. In contrast to pristine Eu_2O_3, the Ti containing honeycomb can easily be resolved in STM.

[1] M. Van den Bossche, J. Goniakowski, and C. Noguera, Nanoscale **13**, 19500 (2021)
[2] P. I. Wemhoff, N. Nilius, C. Noguera, and J. Goniakowski, J. Phys. Chem. C **126** (10), 5070 (2022)

O 14.2 Mon 15:15 H11

Growth of an Fe buckled honeycomb lattice on Be(0001) — Hermann Osterhage[1], Abid H. Khan[2], Karoline Oetker[1], Radek Dao[1], Samaneh Setayandeh[2], Patrick Burr[2], Roland Wiesendanger[1], and •Stefan Krause[1] — [1]University of Hamburg, Germany — [2]University of New South Wales, Sydney, Australia

The Be(0001) surface is considered to be an ideal model system to host a 2D electron gas with pronounced electron-electron and electron-phonon interactions that are decoupled from the bulk [1,2]. In a combined scanning tunneling microscopy (STM) and density functional theory (DFT) study the growth of Fe on a clean Be(0001) surface is investigated on the atomic scale [3]. At low Fe coverage, the nucleation of terraced nanoislands with a disordered surface is observed experimentally with STM. Increasing the Fe coverage results in the growth of extended films exhibiting a well-ordered p(2×2) superstructure. DFT is applied to investigate the growth of Fe on a Be(0001) surface from individual atoms to extended films.

The Fe buckled honeycomb lattice formation on Be(0001), as derived from our study, provides evidence for the realization of a very peculiar non-trivial electronic and magnetic model system. The results will be presented and discussed in terms of their implications for the emergence of novel electronic and magnetic phases resulting from the interactions between the 2D electron gas and the magnetic atoms.

[1] P. T. Sprunger *et al.*, Science **275**, 1764 (1997).
[2] H. Osterhage *et al.*, Phys. Rev. B **103**, 155428 (2021).
[3] H. Osterhage *et al.*, Surf. Sci **752**, 122609 (2025).

O 14.3 Mon 15:30 H11

Electronic structure and edge states in the 2D Kagome lattice Ta_2S_3 / Au(111) — •Thais Chagas[1], Alessia Bardazzi[1], Samuel M. Vasconcelos[2], Alan C. R. Souza[3], Catherine Grover[1], Alice Bremerich[1], Kai Mehlich[1], Daniel Weber[1], Mario S. C. Mazzoni[3], Michael Rohlfing[2], and Carsten Busse[1] — [1]Department Physik, Universität Siegen, Germany — [2]Institute of Solid State Theory, Universität Münster, Germany — [3]Departamento de Física, Universidade Federal de Minas Gerais, Brazil

Kagome structures are a key model system in quantum physics, representing one of the most geometrically frustrated 2D magnetic lattices. In these systems, magnetic moments condense into a spin liquid phase at low temperatures, leading to intriguing physical phenomena. The characteristic Kagome bands in this lattice consist of a Dirac cone that gives rise to massless Dirac fermions with high mobility and a flat band that, in contrast, leads to fermions with infinite effective mass.

In this work, we investigate the 2D Ta_2S_3 Kagome phase on Au(111) using scanning tunneling microscopy (STM). STM images reveal bright island edges as a consequence of an enhanced density of states, indicating the presence of edge states. Additionally, we observe a significant dependence of atomic contrast on tunneling conditions, suggesting a complex electronic band structure near the Fermi level. Furthermore, we analyze the impact of growth parameters on defect formation. Finally, density functional theory (DFT) was employed to study the electronic structure of this material on Au(111), providing deeper insight into its electronic properties and interactions.

O 14.4 Mon 15:45 H11

Spectroscopic and microscopic study of (car)borane based 2D materials — •Martha Frey[1], Julian Picker[1], Jakub Visnak[2], Christof Neumann[1], Tomas Base[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — [2]The Czech Academy of Sciences, Institute of Inorganic Chemistry, 250 68 Husinec-Rez, c.p. 1001, Czech Republic

Boranes are electron-delocalized molecular clusters containing boron and hydrogen. Their electron-deficient bonding and structural diversity as well as their high thermal stability make them attractive for applications ranging from optoelectronics to energy storage. Here we present the fabrication of a novel boron-based, carbon free two-dimensional (2D) material via electron-induced crosslinking of borane-based self-assembled monolayers (SAMs) on silver substrates. The SAMs, crosslinking process and resulting nanomembranes were analyzed using complementary surface-sensitive techniques including X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS), low-energy electron diffraction (LEED) and scanning tunneling and electron microscopies (STM, SEM). Furthermore, the results were compared with carborane-based 2D nanomaterials studied previously in our labs. The results demonstrate that properties of the 2D (car)borane nanosheets can be adjusted and tailored by the respective SAM constituents and that these structurally diverse cluster molecules open up new avenues for engineering novel functional 2D materials.

O 14.5 Mon 16:00 H11

Growth and Structure of Titanium Ditelluride Films on Au(111) — •Andreas Raabgrund, Alexander Wegerich, Lutz Hammer, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Aiming at the MBE growth of transition metal ditelluride (MTe_2) films particularly in the single-layer limit, the formation of and interaction with the interface is of fundamental interest. The growth of a MTe_2 film can be achieved either by the tellurization of the desired metal substrate [1] or by the reactive deposition of Te and the corresponding transition metal M on a suitable substrate [2].

In this contribution we follow the latter approach and investigate both single- and multilayer $TiTe_2$ films on Au(111) by LEED-IV, DFT, and STM. At first glance, LEED suggests a (4×4) superstructure with three $TiTe_2$ on four Au(111) unit cells. STM topography, however, reveals a mismatch of about 1% of the growing film w.r.t. the Au(111) substrate which indicates a relaxed $TiTe_2$ layer. LEED-IV results favor a film in close contact with Au substrate (Te-Au layer distance: ≈ 2.7 Å). By DFT total energy calculations we find that neither Te nor Ti substitution is favored in the topmost Au layer. Continuing the reactive deposition of Ti and Te a multilayer $TiTe_2$ film grows epitaxially as found by LEED-IV with a Pendry R factor of 0.12. Further, we discuss the transferability of this growth recipe to other MTe_2 films on Au(111).

[1] T. Kißlinger et al., Phys. Rev. B **108**, 205412 (2023)
[2] K. Lasek et al., ACS Nano **14**, 8473 (2020)

O 14.6 Mon 16:15 H11

Growth and Edge Reconstruction of 2D MnI_2 on Ag(111) —

•Daniel Rothhardt[1,2,3], Christopher Penschke[4], Hans Josef Hug[1,2], Regina Hoffmann-Vogel[3], and Amina Kimouche[3] — [1]Empa, 8600 Dübendorf, Switzerland — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland — [3]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [4]Institute of Chemistry, University of Potsdam, 14476 Potsdam, Germany

The reduced dimensionality of thin transition metal dihalide films on single-crystal surfaces enables a wide array of magnetic and electronic phenomena. However, producing stoichiometric monolayer islands demands thorough control over growth parameters. In this work, we utilize scanning probe microscopy (SPM) to explore the growth of MnI$_2$ on Ag(111) through single-crucible evaporation. The Ag(111) surface's catalytic activity promotes dehalogenation of MnI$_2$, resulting in a reconstructed iodine adlayer that serves as a template for the formation of truncated hexagonal MnI$_2$ islands. These islands display alter-nating edge lengths and distinctive Kelvin potentials, as revealed by Kelvin Probe Force Microscopy (KPFM). Density Functional Theory (DFT) calculations corroborate the experimental observations, including island heights, lattice parameters, and edge formation energies for both pristine and reconstructed edges. The asymmetry in edge lengths arises from differences in formation energies, determined by the orientation (up or down) of iodine atoms at the edges, as confirmed by DFT.

O 14.7 Mon 16:30 H11

Low defect density in MoS$_2$ monolayers grown on Au(111) by metal-organic chemical vapor deposition — •Julian Picker, Ziyang Gan, Christof Neumann, Antony George, and Andrey Turchanin — Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena, Germany

Monolayers of transition metal dichalcogenides (TMDs) possess high potential for applications in novel electronic and optoelectronic devices and therefore the development of methods for their scalable growth is of high importance. Among different suggested approaches, metal-organic chemical vapor deposition (MOCVD) is the most promising one for technological applications because of its lower growth temperature compared to most other methods, e.g., conventional chemical vapor or atomic layer deposition (CVD, ALD). Here we demonstrate the epitaxial growth of MoS$_2$ monolayers on Au(111) by MOCVD at 450 °C. We confirm the high quality of the grown TMD monolayers down to the atomic scale using several complementary methods. These include Raman spectroscopy, non-contact atomic force microscopy (nc-AFM), X-ray photoelectron spectroscopy and scanning tunneling microscopy (STM). The topographic corrugation of the MoS$_2$ monolayer on Au(111), revealed in a moiré structure, was measured as 20 pm by nc-AFM. The estimated defect density calculated from STM images of the as-grown MoS$_2$ monolayers is in the order of 10^{12} vacancies/cm^2. The defects are mainly caused by single sulfur vacancies.

J. Picker *et al.*, Micron **186**, 103708 (2024).

O 14.8 Mon 16:45 H11

Characterization of a large-scale single-domain MoS$_2$ monolayer — •Fabian Schöttke[1], Luka Pirker[2], Martin Vondráček[3], Michaela Hanušová[2], Václav Valeš[3], Jan Honolka[3], Otakar Frank[2], Matěj Velický[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Münster, Germany — [2]J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Prague, Czech Republic — [3]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

To fully utilize the outstanding optical and electronic properties of single-layer transition metal dichalcogenide (TMDC) in devices, a perfect single-domain film is needed. From the wealth of available preparation methods, exfoliation seems to provide the highest film quality. This method, however, commonly results in small flakes within the micrometer regime only. Exfoliation onto, or assisted by, a Au(111) surface is able to result in large-scale single-domain samples of several millimeters in diameter. We experimentally confirm the high quality of a MoS$_2$ monolayer on Au(111) by characterizing several sample properties: optical appearance, long-range structural order, work function changes, and the occupied & unoccupied electronic structure. Optical inspection and diffraction patterns easily identify millimeter-sized single domains. The electronic structure of MoS$_2$ is clearly distinguished from Au(111) states, especially measured by inverse photoemission in the L gap of Au(111). In summary, our experimental data of a MoS$_2$ monolayer exfoliated onto Au(111) demonstrate the capability of this procedure to produce large-scale single-domain TMDC samples.

O 14.9 Mon 17:00 H11

Kinetics of borophene growth on Ir(111) via boron segregation from the bulk — •Marin Petrović[1], Sherif Kamal[1], Borna Radatović[1], Marko Kralj[1], Matteo Jugovac[2], Iulia Cojocariu[2], Andrea Locatelli[2], and Tevfik Onur Menteş[2] — [1]Centre for Advanced Laser Techniques, Institute of Physics, 10000 Zagreb, Croatia — [2]Elettra - Sincrotrone Trieste S.C.p.A, 34149 Trieste, Italy

Segregation of boron atoms to the Ir(111) surface and their self-assembly into a borophene monolayer were tracked by low-energy electron microscopy (LEEM). Real-time monitoring of sample temperature, boron adatom concentration and borophene coverage reveals the kinetics of boron segregation from the iridium bulk and different modalities of borophene epitaxial growth. It is found that the temperature-triggered boron segregation to the surface is accompanied by instantaneous nucleation of borophene islands and condensation of boron adatoms, followed by rapid propagation of island perimeter along the iridium terraces. Subsequent growth of borophene proceeds by displacement of iridium surface steps, which is energetically expensive and thus relatively slow process that heavily depends on the step morphology. By identifying and analyzing quasi-equilibrium conditions on the sample surface during borophene growth, formation enthalpy of a boron monomer from borophene was estimated, which agrees well with the available theoretical calculations of the boron-iridium system.

O 14.10 Mon 17:15 H11

Growth and etching of hBN on Cu(111): Impact on substrate step dynamics and morphology — •Patrick Seleš[1,2], Marin Petrović[1], Smruti Ranjan Mohanty[3], and Frank Meyer zu Heringdorf[3] — [1]Center for Advanced Laser Techniques, Institute of Physics, Bijenička 46, Zagreb, Croatia — [2]Faculty of physics, University of Rijeka, Radmile Matejčić 2, Rijeka, Croatia — [3]Faculty for Physics, University of Duisburg-Essen, Lotharstrasse 1-21, Duisburg, Germany

The interaction of precursors and oxygen molecules with metal surfaces plays an important role in the growth dynamics of two-dimensional material such as graphene and hexagonal boron nitride (hBN). By using low-energy electron microscopy (LEEM), in this study we investigate the influence of hBN growth on Cu(111) step dynamics at various stages ranging from borazine precursor dosing to oxygen etching. Real-time monitoring of Cu step displacement underneath and next to hBN islands revealed step pinning and a significant decrease in step velocities compared to the pristine Cu surface, highlighting the stabilizing effect of hBN. After the removal of hBN islands by oxygen etching, Cu steps accelerated back to the pre-growth velocities and rearranged into a new surface morphology. Our findings elucidate the interplay between surface dynamics and step motion during hBN growth on Cu(111). By analyzing step displacement and morphological evolution, we contribute to a deeper understanding of metal-catalyzed chemical vapor deposition growth of hBN.

O 14.11 Mon 17:30 H11

In-situ growth and characterization of 2D TaSe$_2$ on Au(111) — •Cathy Sulaiman[1], Lars Buss[1], Raquel Sánchez-Barquilla[1], Jens Falta[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Institute for Solid State Physics, University of Bremen, Bremen, Germany

Group V dichalcogenides such as TaX_2 (X = S, Se, T) have extensively been investigated in recent decades due to their diverse electron correlation effects, including the occurrence of charge density waves and Mott-Hubbard transitions. In 2D, two polytypes, 1T and 1H, exist, which exhibit distinct properties, making selective growth of each polytype crucial. Using low-energy electron microscopy (LEEM), we have successfully observed the growth of two TaSe$_2$ phases on Au(111) *in situ* after the co-deposition of Ta and Se. At elevated temperature, micron-sized, triangle-shaped islands with bright contrast nucleate first and grow at a higher rate. However, this phase turns out to be metastable as it suddenly transitions into a more stable phase (with dark contrast) and continues to grow at a reduced rate. Low-energy electron diffraction shows the presence of TaSe$_2$; bandstructure-sensitive I(V)-LEEM analysis reveals substantial differences in electron reflectivity between both phases. A comparison with TaS$_2$ suggests that the metastable and stable phases are 1T- and 1H-TaSe$_2$, respectively.

O 14.12 Mon 17:45 H11

CVD growth of monolayer transition metal dichalcogenides heterostructures using liquid precursors — •Md Tarik Hossain[1], Axel Printschler[1], Julian Picker[1], Christof Neumann[1], Moritz Quincke[2], Johannes Biskupek[2], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena 07743, Germany — [2]Central Facility of Electron Microscopy, Electron Microscopy Group of Material Science, University of Ulm, Ulm 89081, Germany

Heterostructures (HSs) formed of transition metal dichalcogenide (TMD) monolayers have attracted substantial research interest due to their unique physical properties. However, engineering the HS configurations (lateral and vertical) including the domain size for each TMD remains challenging. Here we present a facile route for the synthesis of different types of HSs of TMD monolayers using liquid precursors for transition metals. We characterized the TMD HSs by several complementary spectroscopy and microscopy techniques. Our results suggest that the HS configurations, lateral length and area of each TMD can be tuned by varying concentration ratios of the precursors. In addition, the overall heterostructure sizes can also be tuned from few to hundreds of micrometers. The developed method paves the way to obtaining high-quality lateral and vertical HS of $MoSe_2$-WSe_2 with controllable domain sizes.