

O 39: 2D Materials III: Growth and Heterostructures (joint session O/HL)

Time: Tuesday 10:30–13:45

Location: GER 38

O 39.1 Tue 10:30 GER 38

High structural and optical quality of transition metal dichalcogenides grown by chemical vapor deposition —

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We have achieved highly reproducible large area growth of high-quality monolayer transition metal dichalcogenides (TMDs) by our modified chemical vapor deposition (CVD) process. We correlate the structure of our CVD grown MoS₂ monolayers studied by high-resolution transmission electron microscopy (HRTEM) with the optical quality revealed in temperature dependent optical spectroscopy. We determine a defect concentration of the order of 10^{13} cm^{-2} for our samples with HRTEM. We show optical transition linewidth of 5 meV at low temperature ($T = 4 \text{ K}$) for the free excitons in emission and absorption after encapsulation in hBN. This is comparable to the best monolayer samples obtained by mechanical exfoliation of bulk material.

O 39.2 Tue 10:45 GER 38

Analysis of Airborne Contamination on Transition Metal Dichalcogenides with Atomic Force Microscopy Revealing That Sulfur Is the Preferred Chalcogen Atom for Devices Made in Ambient Conditions —

KORBINIAN PÜRCKHAUER, •DOMINIK KIRPAL, ALFRED J. WEYMOUTH, and FRANZ J. GIESSIBL — University of Regensburg, Germany

The fabrication of devices incorporating transition metal dichalcogenides (TMDCs) is mostly done in ambient conditions, and thus the investigation of TMDCs cleanliness in air at the nanoscale is important. We imaged MoS₂, WS₂, MoSe₂, and WSe₂ using atomic force microscopy. Mechanical exfoliation of the TMDCs provided clean terraces on sulfides MoS₂ and WS₂. In contrast, the selenides appeared to be contaminated directly after cleavage in most cases. Long-term measurements on MoSe₂ revealed that these unwanted adsorbates are mobile on the surface. In situ cleavage and imaging of WSe₂ in ultra-high vacuum shows clean surfaces, proving the airborne character of the adsorbed particles.

[1] K. Pürckhauer et al., ACS Appl. Nano Mater. 2(5), 2593 (2019)

O 39.3 Tue 11:00 GER 38

Capturing the Carpet Growth of 2D-Silica Films —

•LEONARD GURA, ADRIAN LEANDRO LEWANDOWSKI, ZECHAO YANG, HEINZ JUNKES, MARKUS HEYDE, WOLF-DIETER SCHNEIDER, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Silica films represent a new class of two dimensional (2D) network formers with interesting material properties. To understand the growth process of these van der Waals bound films, we need to understand their mesoscopic structure.

Exfoliation experiments and low energy electron microscopy (LEEM) studies emphasize a smooth and continuous growth of the silica films across single metal crystals [1,2].

In this study, we use scanning tunneling microscopy (STM) to resolve the ring structure of an amorphous silica bilayer film across Ru(0001) step edges. The structural analysis verifies areas of the film with an intact and closed network structure over step edges. The ring sizes are determined with a program for semi-automated ring detection. In this program, we perform a segmentation of the STM image and build a region adjacency graph (RAG) based on the detected ring center coordinates.

We observed areas with carpet growth characteristics in the amorphous 2D-silica film. In future we hope to apply these tools for the detection of structural dynamics as a function of time and temperature.

[1] DOI: 10.1016/B978-0-12-409547-2.14171-X

[2] DOI: 10.1002/anie.201802000

O 39.4 Tue 11:15 GER 38

Where the MoS₂ bilayer grows: An *in situ* LEEM study —

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Molybdenum disulfide (MoS₂) is well-known for changing from an indirect to a direct semiconductor when its thickness is reduced to a single layer, rendering a high degree of growth control a necessity for optoelectronic applications. An extensively investigated model system is MoS₂ on Au(111), which using molecular beam epitaxy typically grows as clusters. Here, we present an in-situ low-energy electron microscopy (LEEM) study of the extended growth of MoS₂ at 700°C and 750°C. These conditions lead to the formation of micron-sized single-layer MoS₂ islands. The single-domain character of these islands is demonstrated by employing dark-field imaging and micro-diffraction (LEED), which allow quantifying the relative coverage of the two mirror domains. Furthermore, selected area angle-resolved photoelectron spectroscopy of these domains directly confirms their threefold symmetric electronic bandstructure. Interestingly, under certain conditions subsequent structural characterization by I(V)-LEEM clearly identifies regions where a bilayer of MoS₂ has nucleated. Parameters influencing the bilayer growth as well as its electronic properties will be discussed.

O 39.5 Tue 11:30 GER 38

Growth of Hexagonal Boron Nitride and Borophene on Ir(111) via Thermal Catalytic Decomposition of Borazine (B₃H₆N₃) —

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Preparation of borophene has been performed by deposition from an e-beam heated high-purity boron rod via molecular beam epitaxy (MBE) [1]. However, the MBE technique is very expensive with low yield and most of all, epitaxially grown borophene islands are found small sized. Here we report on the first successful growth of large area borophene via the thermal catalytic decomposition of borazine (B₃H₆N₃) on a Ir(111) substrate at high temperatures using conventional CVD technique. The observed growth mode is describe to be similar with boron dissolving into the bulk at high temperatures and segregating to the surface forming large borophene sheets as the sample is cooled [1]. The surface morphology and structure determination has been performed in-situ by real-time growth observation via low energy electron microscopy (LEEM) and high-resolution spot profile analyzing-LEED (SPA-LEED). The chemical composition has been determined ex-situ by X-ray photoemission spectroscopy (XPS) and time-of-flight secondary ion mass spectroscopy (ToF-SIMS) measurements. [1] ACS Nano 13, 3816-3822 (2019)

O 39.6 Tue 11:45 GER 38

Electronic properties of coherently attached nanocrystals measured by scanning tunneling spectroscopy —

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2D systems have attracted considerable interest in recent years. The first 2D material was graphene which displays a rich band structure. While it is not possible to create a 2D honeycomb structure with any element we want, artificial lattices emerge as new field to explore. It was shown that it is possible to create superlattices based on semiconductor nanocrystals (PbSe, CdSe) as building blocks in a square and honeycomb geometry. It is of high interest to combine the large scale self-assembly of such superlattices with the possibility of optical and electrical switching. Theoretical works have been initiated based

on tight-binding calculations. Those calculations have shown that the atomic crystalline structure of the nanocrystals combined with the square or honeycomb geometry determine the band structure of the system where Dirac-cones and non-trivial flat bands appear. Until now, the density of states of those structures has not been resolved. In this presentation, I will describe the synthesis and the preparation of the samples and present the measurements of the density of states on PbSe square superlattices by scanning tunneling spectroscopy

O 39.7 Tue 12:00 GER 38

Deconfinement in van der Waals Stacks: Turning Mott Localized Electrons into Dirac Fermions — ●JOSE PIZARRO^{1,2}, SEVERINO ADLER³, KARIM ZANTOUT⁴, THOMAS MERTZ⁴, PAOLO BARONE⁵, ROSER VALENTI⁴, GIORGIO SANGIOVANNI³, and TIM WEHLING^{1,2} — ¹University of Bremen — ²Bremen Center for Computational Material Sciences — ³University of Würzburg — ⁴Goethe University Frankfurt am Main — ⁵CNR-SPIN, Italy

The interplay of topology and electronic correlations forms a rich ground for the realization of exotic states of quantum matter, with an increased importance in emergent flat bands systems in superlattices. Here, we show how strongly correlated spin-orbit coupled Dirac fermions emerge in bilayers of 1T-TaSe₂ and related group V transition metal dichalcogenides. These materials realize the so-called Star-of-David (SoD) charge density wave (CDW) patterns in each layer, where the stacking of the CDW centers defines the symmetry of the resulting superlattice. When the CDW centers are arranged in a honeycomb pattern, the system realizes a generalized Kane-Mele model with a sizable on-site Hubbard interaction U. The iso-electronic series of 1T-TaSe₂, TaS₂, and NbSe₂ traverses a region of the electronic phase diagram where weakly-to-strongly correlated Dirac semimetallic, Mott antiferromagnetic insulating and quantum spin Hall states compete. We show that stacking and relative rotations between the layers as well as perpendicular electric fields affect the emergent correlated Dirac fermions as effective gauge and mass fields, and control their creation, annihilation and topology.

O 39.8 Tue 12:15 GER 38

Proximity-induced superconducting gap in the quantum spin Hall edge state of monolayer WTe₂ — ●FELIX LÜPKE¹, DACEN WATERS¹, SERGIO C. DE LA BARRERA¹, MICHAEL WIDOM¹, DAVID G. MANDRUS^{2,3,4}, JIAQIANG YAN², RANDALL M. FEENSTRA¹, and BENJAMIN M. HUNT¹ — ¹Department of Physics, Carnegie Mellon University, Pittsburgh, PA 15213, USA — ²Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — ³Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996, USA — ⁴Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA

Van der Waals (vdW) heterostructures allow the combination of different material properties, e.g. non-trivial topology and superconductivity in order to create a topological superconducting state. We demonstrate a novel dry-transfer flip technique which we use to place atomically-thin layers of WTe₂, a quantum spin Hall (QSH) system, on NbSe₂, a vdW superconductor, while maintaining atomically clean surfaces and interfaces. Using scanning tunneling microscopy and spectroscopy (STM/STS), we demonstrate the presence of a proximity-induced superconducting gap in the WTe₂ for thicknesses from a monolayer up to 7 crystalline layers. At the edge of the WTe₂ monolayer, we show that the superconducting gap coexists with the characteristic spectroscopic signature of the QSH edge state [1].

[1] F. Lüpke *et al.*, arXiv:1903.00493 (2019)

O 39.9 Tue 12:30 GER 38

MoSe₂-WSe₂ lateral heterostructures grown by chemical vapour deposition — ●EMAD NAJAFIDEHAGHANI¹, ANTONY GEORGE¹, ZIYANG GAN¹, TIBOR LEHNERT², CHRISTOF NEUMANN¹, XINGCHENG LI¹, UTE KAISER², and ANDREY TURCHANIN¹ — ¹Friedrich Schiller University Jena, Institute of Physical Chemistry, D-07743 Jena, Germany — ²Ulm University, Central Facility of Materials Science Electron Microscopy, D-89081 Ulm, Germany

Recently two-dimensional (2D) transition metal dichalcogenides (TMDs) such as MoS₂, WS₂, WSe₂, MoSe₂ etc. attracted great research interest due to their superior electronic and optical properties. They are identified as promising candidates for applications such as ultrathin, transparent and flexible electronics, optoelectronics and sensing. In order to realize advanced device architectures such as p-n junctions, complementary logic devices, ultrathin photovoltaics, etc. it is essential to develop efficient growth strategies

for combining dissimilar monolayer TMDs to form lateral heterostructures. Here we show large area growth of monolayer MoSe₂-WSe₂ lateral heterostructures by our modified chemical vapour deposition (CVD) technique which uses Knudsen type effusion cells for controlled delivery of precursors [1]. The grown monolayer MoSe₂-WSe₂ lateral heterostructures were characterized using complementary microscopic and spectroscopic techniques such as optical microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), Kelvin probe microscopy and high-resolution transmission electron microscopy (HRTEM) to reveal their structural and chemical quality.

O 39.10 Tue 12:45 GER 38

Two-dimensional metal phases and non-stoichiometric phases of transition metal dichalcogenides — ●THOMAS JOSEPH, MAHDI GHORBANI-ASL, and ARKADY KRASHENINNIKOV — Helmholtz-Zentrum Dresden Rossendorf, Bautzner Landstraße 400, Dresden

Changing the stoichiometry of a material in a controllable manner is a powerful tool to tailor the structure and the properties of a compound solid. For example, new morphologies, such as inversion domains with the associated mirror twin boundaries [1] can be produced in 2D transition metal dichalcogenides by sputtering chalcogen atoms using electron beam [1]. Moreover, suspended monolayer Mo membranes were recently fabricated from monolayer MoSe₂ sheets via complete sputtering of Se atoms in a scanning transmission electron microscope [2]. Motivated by these results, we performed first-principles calculations to understand the energetics of 2D phases of binary compounds which can be referred to as strongly non-stoichiometric transition-metal dichalcogenides. We found that other intermediate metallic non-stoichiometric phases, which are energetically more favourable than pure 2D metals [3], can also exist.

[1] Komsa, H.-P. *et al.*; Native Defects in Bulk and Monolayer MoS₂ from First Principles. *Phys. Rev. B* 2015, 91 (12), 125304.

[2] X. Zhao *et al.*; Atom-by-Atom Fabrication of Monolayer Molybdenum Membranes. *Advanced Materials* 2018, 30 (23), 1707281.

[3] T. Joseph *et al.*; Nonstoichiometric Phases of Two-Dimensional Transition-Metal Dichalcogenides: From Chalcogen Vacancies to Pure Metal Membranes. *J. Phys. Chem. Lett.* 2019, 10 (21), 6492.

O 39.11 Tue 13:00 GER 38

Visualization of multifractal superconductivity in a two-dimensional transition metal dichalcogenide in the weak-disorder regime — CARMEN RUBIO-VERDÚ¹, ANTONIO M. GARCÍA-GARCÍA², HYEJIN RYU³, DEUNG-JANG CHOI¹, JAVIER ZALDÍVAR¹, SHUJIE TANG³, BO FAN², ZHI-XUN SHEN⁴, SUNG-KWAN MO³, JOSÉ IGNACIO PASCUAL¹, and ●MIGUEL M. UGEDA⁵ — ¹CIC nanoGUNE, 20018 Donostia-San Sebastián, Spain. — ²Shanghai Center for Complex Physics, Department of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China. — ³Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA. — ⁴Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA. — ⁵Donostia International Physics Center (DIPC), 20018 San Sebastián, Spain.

Here we investigate the impact of multifractality on the superconducting state of a weakly disordered single-layer of NbSe₂ by LT-STM/STS. The SC gap (width, depth and coherence peaks amplitude) shows characteristic spatial single-wavelength modulation coincident with the periodicity of the QPI pattern observed at EF. Spatial inhomogeneity of the SC gap width, which is proportional to the order parameter in the weak-disorder regime, shows a characteristic log-normal statistical distribution as well as a power-law decay of the two-point correlation function, in agreement with our theoretical model. This novel state is universal and governs the properties of even weakly disordered 2D superconductors with SOC.

O 39.12 Tue 13:15 GER 38

Role of dark trions in the optical response of doped atomically thin semiconductors — ●ASHISH ARORA¹, NILS KOLJA WESSLING¹, THORSTEN DEILMANN¹, TILL REICHENAUER¹, PAUL STEEGER¹, PIOTR KOSSACKI², MAREK POTEMSKI^{2,3}, STEFFEN MICHAELIS DE VASCONCELOS¹, MICHAEL ROHLFING¹, and RUDOLF BRATSCHEITSCH¹ — ¹University of Münster, Germany — ²University of Warsaw, Poland — ³Laboratoire National des Champs Magnétiques Intenses, Grenoble, France

We perform absorption and photoluminescence spectroscopy of intravalley and intervalley trions in transition metal dichalcogenide (TMDC) monolayers encapsulated in hBN, depending on temperature

[1]. We find that an interplay between the thermal distribution of bright and dark trions, and their oscillator strengths gives rise to the unique optical response of each monolayer material. The observed trends in our experiments are excellently reproduced using a model based on the Fermi-Dirac distribution of bright and dark trions. Our analysis yields that there is a dark trion 19 meV *below* the lowest energy bright trion in WSe₂ and WS₂. However, in MoSe₂, the dark trion lies 6 meV *above* the bright trion, while it almost coincides in energy with the bright trion in MoS₂. These results are in excellent agreement with our *GW*-BSE *ab-initio* calculations of trions for these materials. Our observations provide a quantitative understanding of the temperature-dependent optical response of TMDCs. [1] Preprint at <https://arxiv.org/abs/1911.06252>

O 39.13 Tue 13:30 GER 38

Excited-State Trions in Monolayer WS₂ — •THORSTEN DEILMANN¹, ASHISH ARORA², TILL REICHENAUER², JOHANNES KERN², STEFFEN MICHAELIS DE VASCONCELLOS², MICHAEL ROHLFING¹, and RUDOLF BRATSCHITSCH² — ¹Institute of Solid State Theory, University of Münster, Germany — ²Institute of Physics and Center for Nanotechnology, University of Münster, Germany

We discover an excited bound three-particle state, the 2s trion, appearing energetically below the 2s exciton in monolayer WS₂, using absorption spectroscopy and *ab initio GW* and Bethe-Salpeter equation calculations [1]. The measured binding energy of the 2s trion (22 meV) is smaller compared to the 1s intravalley and intervalley trions (37 and 31 meV). Our discovery underlines the importance of trions for the entire excitation spectrum of two-dimensional semiconductors. [1] *Phys. Rev. Lett.* **123**, 167401 (2019)