O 91: 2D materials beyond graphene: TMDCs, silicene and relatives III

Time: Thursday 10:30–13:00 Location: MA 043

O 91.1 Thu 10:30 MA 043

Structure and Electronic Properties of Intrinsic Defects in Single Layer Molybdenum Disulfide on Au(111) — •Christian Lotze, Nils Krane, Asieh Yousofnejad, Gael Reecht, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Germany

Transition metal dichalcogenides (TMDCs) are two-dimensional materials with a natural band gap, making them interesting as sensors, solar cells or LEDs. Single layer molybdenum disulfide (MoS_2) is especially interesting, because it provides a direct band gap [1] and a strong spin-splitting of the valence and conduction band.

Here we grow MoS_2 epitaxially on a Au(111) surface as described in [2]. Using combined scanning tunneling/atomic force microscopy (STM/AFM) at low temperatures, we observe different kinds of defects. Particularly prominent are defects, which appear in sizes of several nanometers. NC-AFM reveals an atomically intact surface layer, suggesting that the origin of the defect is located at the gold interface. At these sites, the band gap of MoS_2 is significantly modified, pointing towards quasi-freestanding MoS_2 on a metal substrate [3]. Moreover, we identify single point defects like Mo and S vacancies by STM/AFM and tunneling spectroscopy. The latter two exhibit localized in-gap defect states, which agree well with simulations from density functional theory [4].

[1] Mak *et al.*, PRL **105**, (2010) 136805; [2] Sorensen, *et al.*, ACS Nano **8**, (2014) 6788; [3] Krane, *et al.*, Nano Lett. **16**, (2016) 5163; [4] González, *al.*, Nanotechnology, **27** (2016), 105702

O 91.2 Thu 10:45 MA 043

Structural vs Electronic Effects in the Moiré Pattern of MoS_2 on Au(111) — •Daniela Dombrowski[1,2], Caio Silva[1], Nicolae Atodiresei[3], Wouter Jolie[1,2], Ferdinand Farwick zum Hagen[2], Pardeep Thakur[4], Vasile Caciuc[3], Thomas Michely[2], Stefan Blügel[3], Tien-Lin Lee[4], and Carsten Busse[1,2,5] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [4]Diamond Light Source, United Kingdom — [5]Department Physik, Universität Siegen, Germany

Scanning tunneling microscopy (STM) measurements of molybdenum disulfide (MoS_2) grown on Au(111) show a strong corrugation of the moiré pattern, arising from the lattice mismatch between the MoS_2 layer and the underlying gold substrate. However, STM measurements do not give a pure structural information, since the tip follows the contour of a constant density of states. We combine low temperature scanning tunneling spectroscopy (STS) and x-ray standing wave (XSW) measurements with density functional theory calculations (DFT) to separate structural and electronic contributions to the moiré modulation. Our XSW measurements indicate that MoS_2 on gold is nearly flat in agreement with DFT calculations, giving a corrugation of 0.3 Å. In STS measurements we observe a significant shift of the valence band edge, following the moiré periodicity. This suggests that the observed corrugation in STM has mainly an electronic nature.

O 91.3 Thu 11:00 MA 043

Synthesis and properties of single-layer VS_2 on Au (111) — •Raluca-Maria Stan[1], Fabian Arnold[1], Charlotte Sanders[1], Albert Bruix[1], Sanjoy Mahatha[1], Henriette Lund[1], Maciej Denzik[1], Davide Curcio[1], Harsh Bana[2], Elisabetta Travaglia[2], Luca Bignardi[3], Paolo Lacovig[3], Daniel Lizzit[3], Marco Bianchi[1], Jill Miwa[1], Martin Bremholm[4], Silvano Lizzit[3], and Philip Hofmann[1] — [1]Dep. of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Aarhus, Denmark. — [2]Dep. of Physics, University of Trieste, Trieste, Italy. — [3]Elettra - Sincrotrone Trieste S.C.p.A., Trieste, Italy. — [4]Dep. of Chemistry, University of Aarhus, Aarhus, Denmark.

The single-layer (SL) transitional metal dichalcogenide vanadium disulfide (VS_2) has attracted interest due to predicted intrinsic ferromagnetism that could be exploited in future spintronic applications and data storage devices. For the first time, SL VS_2 of the 1T variety has been synthesized on Au (111). The SL has metallic character and a strong preference to form triangular islands with a moiré superstructure and a well-defined orientation with respect to the substrate. Annealing to temperatures higher than 450 °C, two phase transitions are observed: one phase exhibits a distorted hexagonal unit cell while the other one has a rectangular unit cell characterized by a sulfur deficiency. The unexpected latter phase is reached upon annealing in ultra-high vacuum to temperatures higher than 550 °C. The transition between these phases is reversible upon annealing at lower temperatures in high H_2S pressure.

O 91.4 Thu 11:15 MA 043

Structural and electronic characterization of sulfur depleted monolayer VS2 synthesized on Au(111) — •Umut Kamber[1], Fabian Arnold[2], Brian Kiraly[1], Raluca-Maria Stan[2], Arlette Sohanfo Ngankeu[2], Marco Bianchi[2], Jill Miwa[2], Charlotte Sanders[2], Philip Hofmann[2], and Alexander Ako Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark

Studies on bulk transition metal dichalcogenides (TMDCs) show a variety of electronic properties based on the specific combination of metal and chalcogen elements. Since it is possible to exfoliate or synthesize stable 2D versions of many TMDCs, they have attracted great attention for the opportunity to study reduced dimensionality in a variety of electronic systems. VS2 is of particular interest, as it has not yet been synthesized in monolayer form, and its magnetic ground state is unclear. Here, we present an investigation with low temperature scanning tunneling microscopy/spectroscopy (STM/STS) on the structural and electronic properties of sulfur-depleted single layer VS2 on Au(111). Upon annealing as grown 1T monolayer VS2, there is a structural phase transition to a sulfur depleted phase of VS2, which exhibits reconstructed chain-like structures. Our results shed light on the atomic structure of single layer VS2 as well as reveal a complex Fermi surface of striped phase. STS mapping at low temperature indicates the emergence of non-dispersive electronic ordering close to the Fermi level.

O 91.5 Thu 11:30 MA 043

Bismuth-intercalated WS_2 on Ag(111): a nearly free-standing single-layer TMDC — •Maciej Dendzik[1,2], Sanjoy Mahatha[2], Charlotte Sanders[2], Matteo Michiardi[2,3], Marco Bianchi[2], Jill Miwa[2], and Philip Hofmann[2] — [1]Department of Physical Chemistry, Fritz-Haber-Institut of the Max Planck Society, Faradayweg 4-6, Berlin 14915, Germany — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, BC V6T 1Z1, Canada

Recent developments in the field of two-dimensional transition metal dichalcogenides (TMDCs) have shown that the substrate can have a profound effect on the electronic band structure of these materials [1-3]. For example, a semiconducting single-layer (SL) WS_2 was found to be metallic when grown on Ag(111) [4]. Here we demonstrate that bismuth intercalation can be used to effectively decouple SL WS_2 from the substrate. Angle-resolved photoemission spectroscopy (ARPES) measurements indicate a nearly free-standing character of WS_2 after intercalation. Low-energy electron diffraction (LEED) and scanning-tunneling microscopy (STM) results shed further light on the crystal structure of the investigated WS_2-Bi-Ag complex.

[1] J. A. Miwa *et al.*, Phys. Rev. Lett., **114**, 046802, 2015.
[2] M. Dendzik *et al.*, Phys. Rev. B, **92**, 245442, 2015.
[3] C. E. Sanders *et al.*, Phys. Rev. B, **94**, 081404 (R), 2016.
[4] M. Dendzik *et al.*, Phys. Rev. B, *in press.*

O 91.6 Thu 11:45 MA 043

***In situ* growth and characterization of single-layer molybdenum disulfide on Au(111)** — •Moritz Ewert[1,2], Lars Buss[1], Jens Falta[1,2], and Jan Ingo Flege[1,2] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]MAPEX Center for Materials and Processes, Bremen, Germany

Single-layer (SL) transition metal dichalcogenides are in today's research focus due to their electronic similarity to graphene as well as

owing to their catalytic properties, e. g., in hydrodesulfurization processes.

We have investigated the growth of SL molybdenum disulfide (MoS_2) on Au(111) by Mo metal deposition in dimethyldisulfide background using low-energy electron microscopy (LEEM) and microdiffraction (μLEED). In situ investigations at different elevated temperatures reveal that triangular MoS_2 islands nucleate and continue to grow in a dendritic mode, extending over several square μm in size. The local structure of the islands was elucidated by analyzing the specular electron reflectivity depending on electron energy measurements (IV-LEEM), confirming the sole existence of SL structures. This finding is corroborated by μLEED, which demonstrates the formation of micron-sized MoS_2 SL domains. Furthermore, closer investigation of the mesoscale structure in dark-field LEEM shows that the triangular-shaped structures can be found in two distinct orientations, whose relative abundance has been found to depend on temperature.

O 91.7 Thu 12:00 MA 043

Spin structure of the K valleys in single-layer WS_2 on Au(111) — •Philipp Eickholt[1], Albert Bruix[2], Marcel Holtmann[1], Charlotte Sanders[3], Marko Bianchi[3], Philip Hofmann[3], and Markus Donath[1] — [1]Westfälische-Wilhelms-Universität Münster, Germany — [2]TU München, Germany — [3]Aarhus University, Denmark

In the field of 2D materials, single-layer transition metal dichalcogenides, especially MoS_2, WS_2, $MoSe_2$, and WSe_2, play an important role. Due to their exceptional optical and electronic properties, they are promising materials for optoelectronical applications. The key to understand the material properties is a profound knowledge of the electronic structure. The occupied electronic structure was investigated in a number of studies, yet without spin resolution. In addition, no experimental information concerning band dispersion and spin structure of the conduction bands is available so far.

We present measurements of a combined spin- and angle-resolved direct and inverse photoemission experiment, performed within the same apparatus [1,2]. Our results unravel the spin-dependent energies of the valence- and conduction bands at the K and K' valleys, which are decisive for the optoelectronic properties of the materials.

[1] M. Budke *et al.*, Rev. Sci. Instrum. 78, 113109 (2007)
[2] S.D. Stolwijk *et al.*, Rev. Sci. Instrum. 85, 013306 (2014)

O 91.8 Thu 12:15 MA 043

Pseudodoping of single-layer TaS_2 on Au(111) — Bin Shao[1], •Andreas Eich[2], Charlotte Sanders[3], Arlette Sohanfo Ngankeu[3], Marco Bianchi[3], Philip Hofmann[3], Alexander Ako Khajetoorians[2], and Tim Oliver Wehling[1] — [1]Institut fuer Theoretische Physik (ITP), and Bremen Center for Computational Materials Science (BCCMS), Universitaet Bremen, Germany — [2]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [3]Department of Physics and Astronomy, Interdisciplinary Science Center (iNANO), Aarhus University, Denmark

We demonstrate how weak hybridization of a monolayer of TaS_2 grown on Au(111) can lead to an apparent heavy doping. Combining *ab-initio* calculations and a generic model, we show that strong reshaping of Fermi surfaces and changes in Fermi volumes can arise without actual charge transfer. This mechanism, which we refer to as pseudodoping, explains particular features in the DOS found in the experimental data which are not present in the calculated freestanding case. Moreover, we discuss experimentally observed defects in the TaS_2 monolayer, and illustrate how the changes in hybridization change the experimentally observed features on the LDOS. Finally, we illustrate theoretically that this is a generic effect for metallic 2D materials which are either weakly absorbed to metallic substrates or embedded in vertical heterostructures.

O 91.9 Thu 12:30 MA 043

Synthesis of large area and high-quality MoS_2 monolayers with single domain orientation on Au(111) — Harsh Bana[1], Elisabetta Travaglia[1], •Luca Bignardi[2], Paolo Lacovig[2], Charlotte E. Sanders[3], Maciej Dendzik[3], Matteo Michiardi[3], Marco Bianchi[3], Daniel Lizzit[2], Francesco Presel[1], Dario De Angelis[1], Nicoleta Apostol[4], Pranab Kumar Das[5,6], Jun Fujii[6], Ivana Vobornik[6], Rosanna Larciprete[7], Alessandro Baraldi[1,2,6], Philip Hofmann[3], and Silvano Lizzit[2] — [1]University of Trieste, Trieste, Italy — [2]Elettra Sincrotrone Trieste, Trieste, Italy — [3]University of Aarhus, Aarhus, Denmark — [4]Nat. Inst. Material Physics, Magurele, Romania — [5]Int. Center Theor. Physics, Trieste, Italy — [6]Ist. Officina Materiali-CNR, Trieste, Italy — [7]Ist. Sistemi Complessi-CNR, Rome, Italy

The implementation of MoS_2-based devices exploiting the valley-spin degree of freedom relies on the presence of singly-oriented crystalline domains in the layer, which is not secured by current growth methods. We present a protocol for the synthesis through physical vapor deposition of single-layer (SL) MoS_2 with a single orientation on Au(111) and we characterize the layer with a combination of surface science techniques. Photoelectron diffraction (XPD) proved the single orientation character of the layer, while STM and angular resolved photoemission (ARPES) confirmed the high structural quality. The single domain orientation allowed the measurement, through spin-resolved ARPES, of the complete spin polarization with spin reversal of the states near K and -K points.

O 91.10 Thu 12:45 MA 043

Photocatalytic properties of MoS2 membranes — •Matthias Golibrzuch[1], Elmar Mitterreiter[1,2], Eric Parzinger[1,2], Max Stelzer[3], Franz Kreupl[3], Joel Ager III[4,5], Alexander Holleitner[1,2], and Ursula Wurstbauer[1,2] — [1]Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Am Coulombwall 4a — [3]Department of Hybrid Electronic Systems, Technische Universität München, 80333 München, Germany — [4]Electronic Materials Program, Materials Sciences Division, Lawrence Berkeley National Laboratory — [5]Deptartment of Materials Science and Engineering, University of California, Berkeley, CA 94720

MoS2 is a fascinating two-dimensional van der Waals material with outstanding electronic, optical and catalytic properties. Its high optical absorption up to 15% in the visible range for monolayers together with catalytic activity and photocatalytic stability makes single-layer MoS2 a very promising material for sunlight driven photocatalytic applications such as photocatalytic hydrogen evolution (HER).

We demonstrate the photocatalytic activity regarding HER of exfoliated single- and few-layer MoS2 immersed in an acid electrolyte by cyclic voltammetry. We observe an increased catalytic activity of MoS2 with decreasing number of layers. In particular, monolayers exhibit high current densities, low onset potentials and high turnover frequencies. Edge sites and defects show higher activities than the basal plane. We furthermore demonstrate that HER activity is increased by illumination in the visible range.