O 35: 2D Materials I: Growth and Properties of Transition Metal Dichalcogenides, Phase Transitions

Time: Tuesday 14:00–16:45 Location: H14

O 35.1 Tue 14:00 H14

The unoccupied electronic structure of 2H tungsten disulfide — •Lukas Musiol, Philipp Eickholt, and Markus Donath — Westfälische-Wilhelms-Universität Münster, Germany

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 understanding the material properties is a profound knowledge of the electronic structure. Because freestanding single layers cannot be prepared, experiments are conducted on single layers deposited on a substrate. While the spin structure of the occupied and unoccupied K valleys was investigated for WS_2/Au(111) [1], the influence of the Au(111) substrate is not known in detail.

We present an angle-resolved inverse-photoemission [2,3] study of 2H-WS_2. By comparison with data of single-layer WS_2/Au(111), the influence of the Au(111) substrate is extracted.

[1] P. Eickholt *et al.*, Phys. Rev. Lett. **121**, 136402 (2018)
[2] M. Budke *et al.*, Rev. Sci. Instrum. **78**, 113109 (2007)
[3] S.D. Stolwijk *et al.*, Rev. Sci. Instrum. **85**, 013306 (2014)

O 35.2 Tue 14:15 H14

Charge-transfer across the $MoSe_2$/WSe_2 interface studied with second-harmonic imaging microscopy — •Jonas E. Zimmermann, Ulrich Höfer, and Gerson Mette — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, 35032 Marburg

2D transition metal dichalcogenides (TMDC) have been in the center of attention since the discovery of extraordinary luminescence for MoS_2. TMDC heterostructures in particular gain more and more popularity due to their possible applications in optoelectronics. As the efficiency of such devices is expected to depend strongly on the charge transfer across the heterointerface, it is of crucial importance to investigate the charge-carrier dynamics on a fundamental level.
Here we present results of our second-harmonic (SH) imaging microscopy setup for time-resolved studies on interfaces of 2D materials. This technique enables us to quantify the crystal orientation via polarization dependent measurements and at the same time provides access to the charge-carrier dynamics by femtosecond pump-probe experiments. Measurements performed on MoS_2 monolayers show a strong pump-induced change in the SH response which corresponds well to the fingerprint of exciton generation reported for this material. In contrast, experiments on a $MoSe_2$/WSe_2 heterostructure reveal a delayed filling as well as an enhanced lifetime of the temporal signature. These findings suggest the generation of interlayer excitons in the heterostructure.

O 35.3 Tue 14:30 H14

Phonon dispersion of bulk MoS_2 determined by high resolution electron energy loss spectroscopy — •Holger Schwarz, Christian Heidrich, Florian Speck, and Thomas Seyller — Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany

Transition metal dichalcogenides are currently receiving considerable interest because they are considered as potential building blocks for novel device architectures made up from 2D materials. Basic properties like, e.g. electronic structure as well as phonon and plasmon dispersion, are of fundamental interest in this respect. High resolution electron energy loss spectroscopy (HREELS) is a powerful tool for the investigation of the phononic structure of a solid. Here we use HREELS to study the phonon dispersion of molybdenum disulfide (MoS_2). A clean surface of a MoS_2 bulk crystal was prepared by mechanical cleavage and mild annealing in ultra-high vacuum (UHV). Using low-energy electron diffraction (LEED), the sample was aligned in the high symmetry directions Γ-K and Γ-M, respectively, and subsequent HREELS measurements have been performed in off-specular geometry with a fixed incident electron energy and angle by varying the detector angle of the spectrometer. The spectra were fitted using Voigt-profiles for each resolvable phonon mode. The results are in good agreement with recent DFT-calculations from literature [1] but certain differences in comparison to an earlier HREELS study [2] were noted. [1] A. Molina-Sánchez and L. Wirtz, Phys. Rev. B 84, 155413 (2011) [2] P. A. Bertrand, Phys. Rev. B 44, 5745 (1991)

O 35.4 Tue 14:45 H14

Composition dependence of charge driven phase transition in Group-VI transition metal dichalcogenides from first-principles — Urvesh Patil and •Nuala Mai Caffrey — School of Physics & CRANN, Trinity College, Dublin 2

Atomic intercalation can induce structural phase transitions in a host layered material. For example, group-VI transition metal dichalcogenides (TMDs) are known to undergo a charge-induced phase transition from a semi-conducting H-phase to a metallic T′-phase [1]. The ability to control this phase transition would be advantageous for 2D electronics and catalysis, but it is not well understood, particularly for TMDs beyond MoS_2. Experiment has found that it is comparatively difficult to induce this phase transition in MoS_2 compared to WS_2. However, it is not understood if this can be attributed directly to the electronic properties of these materials, or if the production technique indirectly controls it [2].

Here, we perform a comprehensive side-by-side first-principles investigation of group-VI TMDs (MX_2, where M = Mo, W and X = S, Se), aimed at understanding how alkali metal adsorption affects the phase transition. We show that the barrier for MoS_2 conversion is indeed significantly higher than that of the other TMDs. Finally, we discuss how structural distortions affect the stability of the metallic phase.

[1] Voiry et al, Chemical Society Reviews **44** 2702 (2015)
[2] Ambrosi et al, Chemical Communications **51** 8450 (2015)

O 35.5 Tue 15:00 H14

Observing different levels of airborne contaminations on TMDC materials — •Korbinian Pürckhauer, Dominik Kirpal, Alfred J. Weymouth, and Franz J. Giessibl — University of Regensburg, Regensburg, Germany

The development in nanoelectronics demands reducing the size of its elements which led to an increase of interest in TMDCs. These show a range of interesting properties like a band gap in the range of Si and GaAs and allow high on/off switching ratios for FETs. Fabrication of devices incorporating those TMDCs is mostly done in ambient conditions and thus investigation of TMDCs in ambient is sustainable for the future. We imaged MoS_2, WS_2, $MoSe_2$ and WSe_2 in real space by using atomic force microscopy (AFM). Mechanical exfoliation of the TMDCs provided very large (at least hundreds of nm) clean terraces on MoS_2 and WS_2. In contrast, the $MoSe_2$ and WSe_2 surfaces appeared to be contaminated directly after cleavage in most cases. On all surfaces we were able to observe atomic resolution in ambient conditions. Our findings suggest that TMDCs with sulfur as a chalcogen atom are more suitable for devices made in ambient conditions.

O 35.6 Tue 15:15 H14

Unraveling the growth mechanism of single-domain molybdenum disulfide on Au(111) — •Moritz Ewert[1,2,3], Lars Buss[1,3], Paolo Moras[4], Jens Falta[1,2], and Jan Ingo Flege[1,2,3] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Germany — [3]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [4]Istituto di Struttura della Materia del Consiglio Nazionale delleRicerche, Sincrotrone Trieste SCpA, Italia

As a transition metal dichalcogenide single-layer molybdenum disulfide (MoS_2) is a heavily investigated system. Due to its direct band gap, the electronic properties of single-layer MoS_2 have been subject to several surface science methods. A well-known model system is MoS_2 on Au(111).
We present in situ low-energy electron microscopy (LEEM) and microdiffraction (LEED) observations of MoS_2 growth on Au(111) at elevated temperature using two distinctly different deposition rates. Our investigations reveal similar but different expansion mechanisms of the MoS_2 islands changing a balanced distribution of the two mirror domains towards a single domain distribution. Structural characterization by I(V)-LEEM and investigations of the electronic bandstructure using angle-resolved photoelectron spectroscopy both confirm single-

layer nature of the MoS_2 islands. We could identify step pushing of the growing MoS_2 being responsible for this phenomena.

O 35.7 Tue 15:30 H14

Controlled growth of transition metal dichalcogenide monolayers using Knudsen-type effusion cells for the precursors — •Antony George[1], Christof Neumann[1], David Kaiser[1], Rajeshkumar Mupparapu[1], Tibor Lehnert[2], Uwe Hübner[3], Zian Tang[1], Andreas Winter[1], Ute Kaiser[2], Isabelle Staude[1], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, 07743 Jena, Germany — [2]Ulm University, Central Facility of Materials Science Electron Microscopy, 89081 Ulm, Germany — [3]Leibniz Institute of Photonic Technology, 07745 Jena, Germany

Controlling the flow rate of precursors is essential for the growth of high quality monolayer single crystals of transition metal dichalcogenides (TMDs) by chemical vapor deposition. Thus, introduction of an excess amount of the precursors affects reproducibility of the growth process and results in the formation of TMD multilayers and other unwanted deposits. Here we present a simple method for controlling the precursor flow rates using the Knudsen-type effusion cells. This method results in a highly reproducible growth of large area and high density TMD monolayers. The size of the grown crystals can be adjusted between 10 and 200 μm. We characterized the grown MoS_2 and WS_2 monolayers by optical, atomic force and transmission electron microscopies as well as by Raman and photoluminescence spectroscopies, and by electrical transport measurements showing their high optical and electronic quality based on the single crystalline nature.

O 35.8 Tue 15:45 H14

Reversible crystalline-to-amorphous phase transition in MoS_2 on Gr/Ir(111) by ion irradiation — •Philipp Valerius[1], Joshua Hall[1], Silvan Kretschmer[2], Mahdi Ghorbani-Asl[2], Alexander Grüneis[1], Arkady V. Krasheninnikov[2,3], and Thomas Michely[1] — [1]Universität zu Köln, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]Aalto University, Finland

Grazing incidence 500 eV Xe^+ irradiation transforms a crystalline monolayer of MoS_2 resting on Gr/Ir(111) into an amorphous material as shown by LEED and STM measurements. Moreover, a significant density of states in the band gap evolve, which is evidenced by scanning tunneling spectroscopy. Molecular dynamics simulations uncover that under the irradiation conditions used, sulfur is selectively removed from the top layer, while Mo and the bottom S layer is not sputtered. Through annealing in S vapor, the MoS_2 can be restored as a crystalline semiconductor close to perfection. The structural phase transitions are accompanied by changes in the Raman modes and photoluminescence. As the amorphized MoS_2 monolayer displays metallic properties, selective ion beam amorphization of contact areas could be used as a method to avoid Schottky barriers when contacting MoS_2.

O 35.9 Tue 16:00 H14

Damage mechanisms in two-dimensional MoS_2 under electron irradiation — •Silvan Kretschmer[1] and Arkady Krasheninnikov[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Applied Physics, Aalto University School of Science, Aalto, Finland

Two-dimensional (2D) materials are routinely characterized nowadays in the transmission electron microscope (TEM). The high-energy electron beam in TEM can create defects in the target, and as the influence of defects on materials properties is expected to be stronger in systems with reduced dimensionalities, understanding defect production in 2D materials is of particular importance. Irradiation-induced defects can appear through three mechanisms, namely ballistic or knock-on damage (1), ionization and electronic excitations (2) and beam-induced chemical etching (3). Only the first channel is well understood, while observations of defects formation in 2D transition metal dichalcogenides below the knock-on threshold points out that other mechanism should be important. Here we investigate the role of electronic excitations in defect production by using advanced first-principles simulation techniques based on the Ehrenfest dynamics combined with time-dependent density-functional theory and demonstrate that a combination of excitations and knock-on damage in 2D MoS2 under electron beam can give rise to the formation of vacancies and explain the experimental observations.

O 35.10 Tue 16:15 H14

Nano-patterning of MoS_2 monolayers with focused ion beam — •Rajeshkumar Mupparapu[1], Michael Steinert[1], Antony George[2], Franz Löchner[1], Zian Tang[2], Tobias Bucher[1], Frank Setzpfandt[1], Andrey Turchanin[2], Thomas Pertsch[1], and Isabelle Staude[1] — [1]Institute of Applied Physics, Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena, Germany

Monolayers of transition metal dichalcogenides (TMD-MLs) are immensely interesting for their versatile emission properties [1]. Typically, emission of these extremely thin materials is manipulated either by integrating them on to nanostructures or by assembling into heterostructures. Nano-patterning of TMD-MLs into desired shapes and sizes adds another degree of freedom for their emission manipulation [2, 3]. In this work, we report on nano-patterning of MoS_2 monolayers (MoS_2-MLs) with focused gallium-ion beam while minimizing the damage to the MoS_2 material. To investigate the influence of nano-patterning on emission properties of MoS_2-MLs, we performed photoluminescence, Raman and second harmonic generation measurements. References: [1]. Q. Wang et al., Nat. Nanotech., 7, 699-712 (2012). [2]. W. Guohua et al., Sci. Rep., 7, (2017). [3]. J. Yang et al., Light Sci. Appl., 5, e16046 (2016).

O 35.11 Tue 16:30 H14

Towards Molecular-level Understanding of Ice Nucleation Inhibition at Surfaces — •Naureen Akhtar — Department of Physics and Technology, University of Bergen, P.O. Box 7803, N-5020, Bergen, Norway

The paper that I here submit for the Gerhard Ertl Young Investigator Award presents the first experimental study of the anti-icing properties of graphene and functionalized graphene (fluorinated). The paper demonstrates a completely new approach to anti-icing surfaces, defining a new class of materials, where anti-icing is achieved solely by structuring on the atomic level. The results presented in the paper demonstrate excellent anti-icing performance with freezing delays up to several hours in a high humidity environment. It presents a realistic anti-icing solution that can be implemented in practice. Furthermore the research presented in the paper introduces graphene as a new model-system for understanding ice nucleation mechanism. Finally the results and further work with this new class of material may contribute to the improvement of climate models through the understanding of the role of ice formation in clouds via seeding materials. This is because soot particles are ubiquitous aerosols in the atmosphere and graphene derivatives may serve as suitable model systems, ultimately providing data that can be incorporated in climate models where these effects are currently not taken into consideration.