DS 32: 2D Materials: Growth (Joint session of DS and O, organized by O)

Time: Wednesday 10:30–13:00 Location: S053

DS 32.1 Wed 10:30 S053

Growth and electronic structure of epitaxial single-layer WS_2 on Au(111) — •Maciej Dendzik, Matteo Michiardi, Charlotte Sanders, Marco Bianchi, Jill A. Miwa, Signe S. Grønborg, Jeppe V. Lauritsen, Albert Bruix, Bjørk Hammer, and Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

Single-layer WS_2 is a promising alternative to the widely studied MoS_2, because of the larger size of the spin-splitting and the lower effective mass of the valence band maximum. Here we present a detailed study of the electronic structure of the large-area single-layer WS_2 grown epitaxially on Au(111) using evaporation of W atoms in a low pressure H_2S atmosphere. The growth process is characterized by means of scanning tunneling microscopy, low-energy electron diffraction and core-level spectroscopy. The electronic band structure of the single-layer WS_2 is determined by angle-resolved photoemission spectroscopy. The valence band maximum at $\bar{K}$ is found to be significantly higher than at $\bar{\Gamma}$. The observed dispersion around $\bar{K}$ is in good agreement with density functional theory calculations for a free-standing monolayer, whereas the bands at $\bar{\Gamma}$ are found to be hybridized with states originating from the Au substrate. Strong spin-orbit coupling leads to a large spin-splitting of the bands in the neighborhood of the $\bar{K}$ points, with a maximum splitting of 419(11) meV. The valence band dispersion around $\bar{K}$ is found to be highly anisotropic with spin-branch dependent effective hole masses of $0.40(02)m_e$ and $0.57(09)m_e$ for the upper and lower split valence band, respectively.

DS 32.2 Wed 10:45 S053

Synthesis of high quality TaS_2 monolayer using molecular beam epitaxy — •Arlette S. Ngankeu, Charlotte E. Sanders, Marco Bianchi, Maciej Dendzik, and Philip Hofmann — Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

The transition metal dichalcogenide TaS_2 has been intensively studied in its bulk form due to the rich properties arising from the interplay of electronic instabilities. As in many other materials, the electronic properties of TaS_2 might change in interesting ways in the thickness limit of a single layer. However, finding a good method for the production of high quality single layer TaS_2 is still a big challenge, and the thinnest crystals of TaS_2 obtained so far (by exfoliation of the TaS_2 bulk) actually have thicknesses of a few monolayers. In this talk, we report the first successful preparation of single- and few-layered TaS_2 on the Au(111) substrate by molecular beam epitaxy. Scanning tunneling microscopy, low energy electron diffraction and angle resolved photoemission spectroscopy have been used to probe the surface topography and electronic properties of TaS_2/Au.

DS 32.3 Wed 11:00 S053

2D Heterojunctions from Non-local Manipulations of the Interactions — Malte Rösner[1,2], •Christina Steinke[1,2], Michael Lorke[1], Christopher Gies[1], Frank Jahnke[1], and Tim O. Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany

We propose to create lateral heterojunctions in homogeneous two-dimensional materials based on non-local manipulations of the Coulomb interaction using structured dielectric substrates. By means of ab-initio calculations for MoS_2 as well as generic semiconductor models, we show, that changes in the dielectric environment can induce sizeable band-gap modulations. The Coulomb interaction induced self energy corrections in real space are sufficiently non-local, to be manipulated externally, and are clearly localized within a radius of a few unit cell at the same time. This allows to induce spatially sharp interfaces within a single homogeneous monolayer and thus to form a heterojunction by the external manipulation of the Coulomb interaction via structured dielectric substrates. Hence, new kinds of heterojunctions can be constructed by placing semiconducting 2d materials on appropriately structured substrates: For a laterally structured dielectric environment, we find a type-II heterojunction with a sharp band-gap crossover within less than 5 unit cells. By establishing four perpendicular interfaces a band gap modulation reminiscent of a quantum dot can be realised.

DS 32.4 Wed 11:15 S053

TFT Fabrication Based on Liquid Exfoliated MoS_2 Flakes — •Xiaoling Zeng[1], Sonia Metel[2,3], Valeria Nicolosi[2,3,4], and Veit Wagner[1] — [1]Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany — [2]School of Chemistry, Trinity College Dublin, Ireland — [3]CRANN, Trinity College Dublin, Ireland — [4]School of Physics, Trinity College Dublin, Ireland

There is a large interest in establishing cheap, scalable processes for producing low dimensional semiconducting dichalcogenide films for electronic application. In this work, well exfoliated MoS_2 dispersions were prepared through two step liquid phase exfoliation process with N-methyl-pyrrolidone (NMP) and Isopropanol (IPA). The obtained exfoliated MoS_2 flakes were characterized by microscopy (TEM and SEM), Uv - Vis and Raman spectroscopy.

Bottom gate thin film transistors (TFTs) based on exfoliated MoS_2 film were fabricated by using spray coating techniques. The deposition process was optimized to get uniform and percolated MoS_2 film with different thicknesses. Transistors show only minor conductivity directly after layer deposition. However, depositing additional PMMA layer on top shows large improvement in electrical characteristics, i.e. switching behavior with changing gate voltage. Interpretation is that the PMMA layer brings the initially separated flakes into contact and enables proper percolation. Further investigation found that the thickness of PMMA influences the electrical properties. This low-cost and scalable solution-based fabrication process will promote the application of dichalcogenides in future nanoelectronic devices.

DS 32.5 Wed 11:30 S053

Novel Deposition Approach of Semiconducting MoS2 Thin Films and Their Application for Electronic Devices — •Francis Oliver Vinay Gomes[1,2], Marko Marinkovic[1], Jochen Brendt[1], Torsten Balster[2], and Veit Wagner[2] — [1]Evonik Resource Efficiency GmbH, Paul-Baumann-Strasse 1, 45764 Marl, Germany — [2]Jacobs University Bremen, Department of Physics & Earth Science, Campus Ring 1, 28759 Bremen, Germany

In this work, MoS2 films obtained from precursor solution via spin-coating on various substrates were investigated. Molybdenum(V) chloride dissolved in 1-methoxy-2-propanol was used as precursor solution. The MoS2 films obtained from the Mo-precursor upon sulfurization during annealing were analyzed for surface morphology and roughness, chemical composition and crystallinity. In addition, comparison of silicon and sapphire substrates were studied. Our approach focuses on novel deposition technique compared to the current state-of-the-art chemical vapour deposition.

The thickness of the MoS2 films was controlled in the process, and film thicknesses between 2 and 27 nm were obtained. The thickness of the films linearly scaled with precursor concentration. SEM/EDX measurements indicate that the surface morphology and film composition is strongly dependent on the annealing temperature and processing environment. Electrical measurements demonstrate a film conductivity of 0.27 S/cm while XRD confirms the formation of semiconducting 2H-MoS2 films. The future steps will lead towards applying fabricated films in electronic devices such as thin film transistors.

DS 32.6 Wed 11:45 S053

Growing graphene underneath hBN on Rh(111) — •Uta Schlickum[1], Daniel Rosenblatt[1], Sebastian Koslowski[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The stable hexagonal monolayer of hBN is an insulator with excellent dielectric properties. It can be grown on a large variety of transition metal surfaces like Rh(111) on which it shows a hexagonal Moire super-lattice. We grow a single layer of hBN on Rh(111) by chemical vapor deposition and found beside the well known hexagonal structure a new periodic pattern resembling a lattice of a "spoked wheel" (SW). For small coverages this new phase appears at the intersection of the rims connecting three valleys of the Moire lattice, and forms

large islands for higher coverage. Atomic resolution topographic images reveal that the phase boundaries do not disturb the atomic lattice periodicity of the hBN. Depending on the preparation parameters, the relative coverage of the two phases can be tuned at will. The crucial parameter determining the relative coverage is the time, the sample stays at about $600°C$ after the exposure to borazine at $800°C$. It is well known that at $600°C$, C impurities segregate and accumulate at the surface. This together with the fact that the hBN lattice itself remains intact crossing a phase boundary, leads us to conclude that the SW phase consists of an additional graphene layer below the hBN layer. Various experimental details, like high resolution spectroscopy, support this interpretation.

DS 32.7 Wed 12:00 S053

Prediction of metastable two-dimensional compounds in the C/Si system using global optimization techniques, and investigation of their electronic properties — •Johann Christian Schön and Rico Gutzler — MPI for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart

We employ the global energy landscape exploration package G42+[1,2] to predict (meta)stable two-dimensional crystalline polymorphs in the carbon/silicon system for a range of compositions: C:Si = 1:0, 3:1, 2:1, 1:1, 1:2, 1:3, and 0:1.[1] During the global search (energy function: DFT), both atom positions and cell parameters in the xy-plane were allowed to vary freely. The global optimization method used was basin-hopping-simulated annealing, with two consecutive local optimizations - the first keeping the atoms restricted to the z = 0 plane, while the second one also permitted relaxation in the z-direction. For all compositions, the lowest energy 2D-structures exhibited a graphene-like super-structure with 6-membered rings, but many quite stable competing minimum structures containing a variety of rings of size 4 - 12 were also observed. Deviations from planarity occurred most frequently for structures where a high local concentration of the Si-atoms was present. Complementing geometric structure prediction, we performed band-structure calculations to investigate the effect of geometry and C:Si ratio on the electronic properties of these 2D-materials.

[1] J. C. Schön, Proc. Appl. Ceram. 9:157-168 (2015); [2] J. C. Schön, G42+ Manual, www.chemie.uni-bonn.de/ac/schoen/forschung/g42-manual, (2015)

DS 32.8 Wed 12:15 S053

Tuning the physical properties of MoS_2 membranes by organophosphonate interfacial chemistry — •Susanne Schwarzwälder[1], Réka Csiki[1], Eric Parzinger[1], Jeffrey Schwartz[2], Alexander Holleitner[1], Martin Stutzmann[1], Ursula Wurstbauer[1], and Anna Cattani-Scholz[1] — [1]Walter Schottky Institut and Physik Department, Technische Universität München, Germany — [2]Princeton University, New Jersey, USA

One of the most prominent members of the 2D material family is the transition metal dichalcogenide MoS_2, due to its natural occurrence and its promising potential applications in nanoelectronic and optoelectronic devices [1]. Interfacial chemistry strongly influences the interaction of molecularly thin semiconducting membranes with the underlying substrate, hence a suitable silicon surface functionalization can be employed for improving the performance of MoS_2-based devices [2]. Our work focuses on the investigation of surface functionalization using homogeneous organophosphonate self-assembled monolayers (SAMs) covalently bonded to SiO_2. In particular, the interaction of single layer (SL) MoS_2 with SAMs based on four different aromatic phosphonic acids are investigated. Modulation of the intrinsic n-type doping of SL-MoS_2 via charge transfer with aromatic SAMs is suggested by a shift in the Raman-active out-of plane vibrational mode A_{1g}, emphasizing the importance of interfacial interactions in MoS_2-based nanodevices.

[1] R. Ganatra, Q. Zhang, ACS Nano 8, 4074 (2014).
[2] S. Najmaei et al., Nano Lett. 14, 1354 (2014).

DS 32.9 Wed 12:30 S053

Structural analysis of one monolayer of hBN on Cu(111) via NIXSW and SPA-LEED — •Timo Heepenstrick[1], Christine Brülke[1], Ina Krieger[1], Sergey Subach[2], Simon Weiss[2], Niklas Humberg[1], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52452 Jülich, Germany

We present a detailed structural analysis of hBN on Cu(111) with normal incidence x-ray standing waves (NIXSW) supported by spot profile analysis low energy electron diffraction (SPA-LEED). hBN forms an incommensurate structure on Cu(111) with a lattice mismatch of 2.3% corresponding to the unstrained hBN layer. The NIXSW experiments show that the hBN layer is weakly bonded with a distance of 3.23 Å (for the nitrogen) and 3.26 Å (for the boron) and shows little buckling. We also present an analysis for the topmost Cu(111) layer with and without a monolayer of hBN.

DS 32.10 Wed 12:45 S053

Nanotents - 2 nm void-formation and self-healing in 2D monolayers on metals — •Huanyao Cun[1], Marcella Iannuzzi[2], Adrian Hemmi[1], Silvan Roth[1], Jürg Osterwalder[1], and Thomas Greber[1] — [1]Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [2]Chemistry-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

At room temperature, it is quite challenging to immobilize single atoms. However, with the single layers of hexagonal boron nitride (h-BN) or graphene, site-selective immobilization of atoms at surfaces becomes feasible. The h-BN nanomesh is a corrugated structure that consists of two regions, the 'pores' with 2 nm diameter and the surrounding 'wire' regions.

In the present study, we demonstrate that the h-BN nanomesh, which acts as thin "rainfly", can trap atoms at distinct subsurface sites and form so-called "nanotents" structure. Remarkably, annealing to 900 K induces the "can-opener" effect: h-BN flakes at pore sites are cut out from the h-BN monolayer and 2 nm voids form on the h-BN surface. We assign the "can-opener" effect to the vacancy defects generated during the Ar+ penetration. Higher temperature annealing leads to the "self-healing" of the h-BN monolayer. Systematic measurements reveal that the entire process, including nanotent formation, "can-opener" effect and nanomesh "self-healing", is well controlled and repeatable. The reported effects are robust and quite general: they are also observed in graphene on ruthenium, for neon and rubidium atoms.