O 46: 2D Materials beyond Graphene: TMDCs, Slicene and Relatives

Time: Tuesday 18:15–20:30 Location: Poster E

O 46.1 Tue 18:15 Poster E

Growth and Characterization of Thin MoS_2 Films on the Buffer Layer on SiC(0001) — •Adrian Schütze[1], Martina Wanke[1], Florian Speck[1], Ovidiu Gordan[2], Gregor Nordheim[1], Thomas Seyller[1], and Dietrich R. T. Zahn[2] — [1]Professur für Technische Physik, TU Chemnitz, Germany — [2]Professur für Halbleiterphysik, TU Chemnitz, Germany

Layered 2D metal dichalcogenides such as MoS_2 are semiconductors with the unique property to transform from an indirect to a direct semiconductor depending on the number of layers. As such they are offering new possibilities for electronic applications. In this work, we study the large-scale chemical vapor deposition of thin layers of MoS_2 on the so-called buffer layer on SiC(0001), a graphene-like reconstruction with covalent bonds to the SiC substrate [1]. The buffer layer was grown in Ar at atmospheric pressure as described elsewhere [2]. MoS_2 was synthesized from $MoCl_5$ and sulfur powder [3] with Ar as carrier gas. X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM) and low-energy electron diffraction were used to characterize the chemical composition and structure of the samples. The thickness of the deposited MoS_2 is estimated to approximately 2 or 3 monolayers from XPS spectra and compared to Raman spectroscopy and AFM results. In addition, XPS data suggesting sulfur intercalation of the buffer layer during the CVD process are presented.

[1] K.V. Emtsev et al., Phys. Rev. B **77**, 155303 (2008).
[2] M. Ostler et al., Phys. Status Solidi B **247**, 2924 (2010).
[3] Y. Yu et al., Sci. Rep. **3**, 1866 (2013).

O 46.2 Tue 18:15 Poster E

Characterization of few layer MoS_2 on Silicon Carbide with Raman Spectroscopy — •Lisa Seitz[1], Adrian Schütze[2], Gregor Nordheim[2], Thomas Seyller[2], and Martin Hundhausen[1] — [1]Lehrstuhl für Laserphysik, FAU Erlangen-Nürnberg — [2]Professur für Technische Physik, Technische Universität Chemnitz

MoS_2 is a layered crystal with electronic properties that depend significantly on the number of layers. Here, we employ Raman spectroscopy for a mapping of layer number and homogeneity of few layer MoS_2, synthesized by CVD on silicon carbide (SiC). The frequencies of the E^1_{2g} and A_{1g} phonon modes depend on the layer number, so that the difference between these frequencies can be used as an indicator of layer number. [1] Different samples were studied by a Raman mapping: One sample shows a domain structure of terraces covered with bi- and trilayer MoS_2, coexisting with clean surface domains. Another sample shows a rather homogeneous coverage of MoS_2 with a layer number of around four to five.

[1] J. Jeon et al., Nanoscale **7**, 1688 (2015).

O 46.3 Tue 18:15 Poster E

Raman- and Photoluminescence Spectroscopy on few- and monolayered WSe_2 — •Walter Enns[1], Sergej Neb[1], Sebastian Fiechter[2], and Walter Pfeiffer[1] — [1]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Helmholtz Zentrum Berlin, Institut für Solare Brennstoffe, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The transition-metal dichalcogenide WSe_2 was exfoliated onto thermal oxidized silicon with 70 nm oxide thickness. Few- and monolayered flakes were investigated with confocal micro-Raman spectroscopy and photoluminescence spectroscopy applying two different wavelengths, 473 nm and 633 nm. The former measures the layer-dependent frequency difference of the out-of-plane to the in-plane vibration, while the latter is sensitive to the typical transition from indirect to direct band gap when changing from few-layer to monolayer WSe_2. Thus, both methods have the capability to distinguish between varying numbers of layers.

O 46.4 Tue 18:15 Poster E

Single-Layer MoS2 on Au(111): Electronic structure — Albert Bruix[1], Jill A. Miwa[1], •Nadine Hauptmann[2], Søren Ulstrup[1], Signe G. Grønborg[1], Charlotte E. Sanders[1], Maciej Dendzik[1], Antonija Grubišić Čabo[1], Marco Bianchi[1], Jeppe Vang Lauritsen[1], Daniel Wegner[2], Alexander A. Khajetoorians[2], Bjørk Hammer[1], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark — [2]Institute for Molecules and Materials, Radboud University, 6500 GL Nijmegen, The Netherlands

Single layer transition metal dichalcogenides are currently of considerable interest because they are 2D materials, like graphene, but have an inherent band gap. Their physical properties, e.g. their band gap and electronic structure, change dramatically in the single layer limit and depend on the underlying substrate. Molybdenum disulfide (MoS_2) as a single layer has already been used in applications such as field effect transistors and optoelectronic devices. We investigate epitaxial single-layer MoS_2 grown on Au(111) by low temperature scanning tunneling microscopy. Using scanning tunneling spectroscopy, we determine the single-particle band gap and compare it to density functional theory calculations of the electronic structure around the Fermi energy in the filled and empty states. At small energies, a low conductance regime is found while for higher energies onsets in the conductance are observed. These onsets are further compared to angle-resolved photoemission spectroscopy data from the same sample.

O 46.5 Tue 18:15 Poster E

Structure and Electronic Properties of MoS_2 on Au(111) — •Nils Krane, Christian Lotze, Julia Läger, Gaël Reecht, and Katharina J. Franke — Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMCD) are two-dimensional materials with a natural band gap, making them interesting as sensors, solar cells or LEDs. Single layer molybdenum disulfide 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 a combined STM/AFM at low temperatures, we observe different kinds of defects. Particularly prominent are defects, which appear in sizes of several nanometers. The AFM reveals an atomically intact surface layer, suggesting that the origin of the defect is located at the gold interface. At these sites the bandgap of MoS_2 is significantly modified.

[1] Mak *et al.*, PRL 105, 136805 (2010)
[2] Sorensen, et al., ACS Nano 8, 6788-6796 2014

O 46.6 Tue 18:15 Poster E

Monolayer epitaxial hexagonal boron nitride on Ir(111) functionalization by caesium adsorption and intercalation — •Jiaqi Cai[1,2], Wouter Jolie[2], Caio Silva[1], Christoph Schlueter[3], Marin Petrovic[3], Marko Kralj[4], Tien-Lin Lee[4], and Carsten Busse[1,2] — [1]Institut für Materialphysik, Münster, Germany — [2]II. Physikalisches Institut, Köln, Germany — [3]Diamond Light Source Ltd, Didcot, United Kingdom — [4]Institut za fiziku, Zagreb, Croatia

Being a wide band gap insulator, hexagonal boron nitride monolayer (hBN) is an important member of the two-dimensional-material family. However, detailed information on the band structure remains unclear. In this respect, adsorption and intercalation of alkali metal on epitaxial hBN are easy routes to investigate its electronic structure.

Here, we report our study on caesium deposition on hBN/Ir(111). Scanning tunneling microscopy/spectroscopy (STM/STS), x-ray photoelectron spectroscopy (XPS), x-ray standing waves (XSW), and angle-resolved photoemission spectroscopy (ARPES) techniques are used to study the morphological and electronic properties of the system. The density and location of caesium (intercalated or adsorbed) varies when different deposition conditions are applied. Accordingly, different shifts of the hBN electronic bands occur in different caesium configurations. The largest shift towards higher binding energy obtained is 3.63 eV. Meanwhile no sign of the conduction band is observed in the ARPES results. This shows hBN has a band gap larger than 5.95 eV.

O 46.7 Tue 18:15 Poster E

Structural Analysis of one monolayer hBN on Cu(111) via SPA-LEED and NIXSW — •Christine Brülke[1], Niklas Humberg[1], Timo Heepenstrick[1], Ina Krieger[1], Simon Weiss[2], Sergey Subach[2], 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

Thin films of hexagonal boron nitride (hBN) are of high interest as an insulating material as well as a template for the formation of highly defined structures of organic molecules. Here, we report a detailed structural analysis of the hBN monolayer on the Cu(111) surface by spot profile analysis low energy electron diffraction (SPA-LEED) and normal incidence x-ray standing waves (NIXSW). hBN grows on the Cu(111) surface in an incommensurate structure with a lattice mismatch of 2.3 % corresponding to an unstrained hBN layer and a domain size of up to 170 Å. The films show rotational mosaicity, however, the majority of the hBN domains are in or close to alignment with the unit cell vectors of the Cu(111) surface. The highly resolved SPA-LEED patterns show detailed structures which can be explained entirely by multiple electron scattering. Both SPA-LEED and NIXSW experiments show that the hBN layer lies topologically flat on the copper surface. The average distance between adsorbate atoms and the first Cu layer is 3.24 ± 0.01 Å. We discuss our results in relation to previous studies.

O 46.8 Tue 18:15 Poster E

Hydrogenation and dehydrogenation of hexagonal - Boron Nitride (h-BN) on Ni(111) — •Florian Späth, Fabian Düll, Christoph Gleichweit, Udo Bauer, Philipp Bachmann, Christian Papp, and Hans-Peter Steinrück — Friedrich-Alexander-Universität, Erlangen-Nürnberg, Germany

Hexagonal-Boron Nitride (h-BN), which is a single atom thick sheet of alternatingly, hexagonal-arranged boron and nitrogen atoms, may be a suitable candidate for future hydrogen storage applications. Here, we investigate its reactivity towards atomic hydrogen, i.e. the hydrogenation, and subsequently the thermally activated dehydrogenation. The system is investigated with high-resolution temperature programmed X-ray photoelectron spectroscopy (HR-XPS) and temperature programmed desorption (TPD). h-BN is prepared via chemical vapor deposition of Borazine (B3N3H6) on a Ni(111) single crystal and subsequently exposed to atomic hydrogen at low temperatures. In HR-XPS, we find distinct chemical shifts after exposure to atomic hydrogen. In the temperature programmed investigation, we observe different dehydrogenation steps occurring at different temperatures, which depend on the initial hydrogen coverage. A comparison to the hydrogenation of graphene on Ni(111) will be shown. We acknowledge the support by the Cluster of Excellence "EAM" and the SFB 953 "Synthetic Carbon Allotropes".

O 46.9 Tue 18:15 Poster E

Epitaxial growth of Sn on SiC(0001): A study by scanning tunneling microscopy — •Felix Reis, Maximilian Bauernfeind, Ralph Claessen, and Jörg Schäfer — Physikalisches Institut, Universität Würzburg

This work is motivated by the unusual properties of graphene, which was the first material predicted to show the quantum spin Hall effect based on its spin-polarized topological edge states, which are located in the bulk energy gap. However, this gap is very small (order of μeV), such that it is impossible to access the edge channels in experiment.

One approach to overcome this problem is to pursue the realization of honeycomb lattices with high-Z atoms. A material that received great attention by theoretical modeling is (free-standing) stanene, made of Sn atoms and predicted to have a significantly larger bandgap due to stronger spin-orbit interaction [1]. However, a substrate – as needed for real-world experiments – had not been considered.

Here we report on the epitaxial growth of Sn reconstructions on SiC(0001) in the regime of around one monolayer coverage. The structures are examined by scanning tunneling microscopy (STM) and low-energy electron diffraction. We observe the formation of long-range ordered Sn-induced atomic lattices. Interestingly, depending on the coverage, these exhibit (3×3) or $(6\sqrt{3} \times \sqrt{3})$ superstructures, respectively. Close-up inspection is suggestive of hexagonal structural units. We will present a detailed analysis of the STM results, and discuss these in the light of theoretical predictions.

[1] Y. Xu *et al.*, Phys. Rev. Lett. **111**, 136804 (2013).

O 46.10 Tue 18:15 Poster E

Synthesis and Electronic Structure of Single-Crystal FeSe on Bi$_2$Se$_3$ — •Charlotte Sanders[1], Nils Rollfing[2], Andreas Eich[2], Fabian Arnold[1], Pascal Ewen[2], Marco Bianchi[1], Maciej Dendzik[1], Matteo Michiardi[1], Daniel Wegner[2], Philip Hofmann[1], and Alexander Ako Khajetoorians[2] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark — [2]Institute for Molecules and Materials, Radboud University, 6500 GL Nijmegen, Netherlands

Single-layer FeSe on SrTiO$_3$ exhibits a superconducting transition temperature T_c that is greatly enhanced over that of bulk FeSe. This fact—which is due, in part, to complex physics at the interface of these two materials—raises the question of whether interesting effects can be realised at the interfaces between FeSe and other types of substrates. Recent work has begun to elucidate the structure and electronic properties of single-crystal FeSe islands grown on the topological insulator Bi$_2$Se$_3$. Here we extend this line of investigation, combining scanning tunnelling microscopy and low-energy electron diffraction with a detailed mapping of the band structure using angle-resolved photoemission spectroscopy. Remarkably, our findings indicate persistence of the Dirac cone at the FeSe-Bi$_2$Se$_3$ interface. We do not observe superconductivity at temperatures down to 4.7K.

O 46.11 Tue 18:15 Poster E

Photoelectron Spectroscopy On Ferecrystalline Compounds — •Fabian Göhler[1], Gavin Mitchson[2], Matti Alemayehu[2], Christian Raidel[1], Florian Speck[1], David C. Johnson[2], and Thomas Seyller[1] — [1]Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany — [2]Department of Chemistry and Materials Science Institute, University of Oregon, Eugene, Oregon 97403, United States

Ever since the groundbreaking work on graphene by Novoselov and Geim, the preparation and properties of 2D materials have been of great interest to scientists. Going forward, the stacking of different sheet-like materials opens up new ways to design materials with specific properties. Recently, a new class of layered intergrowth materials built up from metal monochalcogenides and transition metal dichalcogenides has been prepared by the method of modulated elemental reactants (MER)[1]. These intergrowths have been termed *ferecrystals*[2], due to the turbostratic disorder occuring between the otherwise perfectly stacked layers.

Herein, we report the results of X-ray photoelectron spectroscopy studies carried out on (MSe)$_1$(NbSe$_2$)$_2$ ferecrystals, where M = Pb, Sn or Bi. Core level and valence band spectra of ferecrystals are compared to the MER-produced binary compounds of MSe and NbSe$_2$, respectively, to investigate inter-layer charge transfer in the ferecrystals.

[1] D. C. Johnson, *Curr. Opin. Solid State Mater. Sci.* **3**, 159 (1998).

[2] M. Beekman et al, *Semicond. Sci. Technol.* **29**, 064012 (2014).

O 46.12 Tue 18:15 Poster E

Angle-resolved photoemission spectroscopy of the possible chiral charge-density-wave state of 1*T*-TiSe$_2$ — •Sascha Beier, Matthias Kallaene, Arndt Quer, and Kai Rossnagel — Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany

The layered transition-metal dichalcogenide 1T-TiSe$_2$ undergoes a transition into a commensurate $2 \times 2 \times 2$ triple-q charge-density-wave (CDW) state at a temperature of ≈ 200 K. Recently, Ishioka *et al.* discovered a possible chiral CDW phase employing scanning tunneling microscopy (STM) below 85 K. Castellan *et al.* determined the transition temperature to this chiral CDW phase to be 7 K below the transition temperature into the normal CDW phase by specific heat, electrical transport properties, and X-ray diffraction measurements. However, a recent STM study questions the existence of an intrinsically chiral CDW state. Novello *et al.* rather attribute the effect to native lattice defects and the substitution of atoms.

Here we present angle-resolved photoelectron spectroscopy (ARPES) data on 1T-TiSe$_2$ utilizing circular polarized synchrotron radiation. In the CDW phase, the electronic structure is characterized by a strong backfolding of the Se 4p-derived bands to the L-point. Dichroism ARPES measurements of this spectroscopic order parameter at the L point apper to be consistent with the emergence of a chiral CDW state at temperatures below 190 K, in good agreement with the results of Castellan *et al.*