O 66: Poster Wednesday: 2D Materials

Time: Wednesday 17:45–20:00 Location: Poster B2

O 66.1 Wed 17:45 Poster B2

Structure formation and electron dynamics of Pb intercalated graphene/metal interfaces — •Eva Sophia Walther[1], Christina Schott[1], Florian Haag[1,2], Dominik Jungkenn[1], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern — [2]Material Science in Mainz, JGU Mainz

Graphene is the most intriguing low dimensional material for future nano-electronics mainly due to its exceptional electronic properties with a Dirac cone-like spectrum and massless Dirac-Fermions. Yet, for electronic devices, it is necessary to find new ways to functionalize the electronic properties of graphene. One promising route to chemically manipulate graphene is the intercalation of heavy metal atoms between the graphene and the underlying substrate surface. This procedure cannot only suppress the interaction between the substrate surface and the graphene sheet but can also lead to the formation of a band gap at the Dirac-point [1]. Here, we present structural changes of the graphene/metal interfaces upon the adsorption and intercalation of Pb atoms using low energy electron diffraction and photoemission electron microscopy. Subsequently, we turn to the electron dynamics in this material system which was investigated by momentum-resolved photoemission spectroscopy. Our results allow us to correlate the electron dynamics to the vertical interactions of the graphene/metal interface prior to and after the adsorption Pb atoms. [1]I.I. Klimovskikh et al. ACS Nano 2017, 11, 368-376

O 66.2 Wed 17:45 Poster B2

A HR-XPS study of the formation of h-BN on Ni(111) from the two precursors, ammonia borane and borazine — •Philipp Bachmann, Fabian Düll, Florian Späth, Udo Bauer, Hans-Peter Steinrück, and Christian Papp — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen, Germany

Together with borazine, ammonia borane is a prominent precursor molecule for the formation of hexagonal boron nitride, which is of high interest as a 2D-material and graphene analog. Ammonia borane is also a possible solid hydrogen carrier with high storage density. Using X-ray photoelectron spectroscopy and temperature-programmed desorption, we investigated low-temperature adsorption and dehydrogenation during heating of borazine and ammonia borane on Ni(111) to form h-BN. For borazine, we observe the formation of disordered boron nitride above 300 K, which starts to form hexagonal boron nitride above 600 K. Ammonia borane shows multiple dehydrogenation steps at the boron and nitrogen atoms up to 300 K. This results in various BHxNHy species, including borazine-like intermediates, before the formation of disordered boron nitride and finally hexagonal boron nitride, analogous to the borazine decomposition. We acknowledge the SFB 953 "Synthetic Carbon Allotropes" for financial support.

O 66.3 Wed 17:45 Poster B2

Mechanical characterization of carbon nanomembranes and graphene via AFM nanoindentation and bulge testing — •Florian Paneff[1], Xianghui Zhang[1], Nikolaus Meyerbröker[2], and Armin Gölzhäuser[1] — [1]Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — [2]CNM Technologies GmbH, 33609 Bielefeld, Germany

With the development of freestanding two-dimensional materials and nanomembranes, the precise characterization of the mechanical properties of these sheets has become an important challenge. It is thus beneficial to combine several methods to obtain more accurate results. Here we employed both bulge testing and nanoindentation performed in an atomic force microscope (AFM) to determine the elastic properties of these nanomembranes. In the former case a uniform pressure was applied to a membrane and the resultant deflection was recorded by the AFM, whereas in the latter case the AFM tip was positioned to the center of the same membrane and force-displacement curves were measured. Both pressure-deflection and force-displacement data were processed and compared with finite element method to determine the elastic properties of the membrane. In this contribution we will report the mechanical properties of carbon nanomembranes prepared from aromatic self-assembled monolayers via electron irradiation. Mechanical characterization of other nanomaterials, such as mono- and bi-layer CVD graphene, carbon nanosheets and pyrolized graphitic carbon, will also be discussed.

O 66.4 Wed 17:45 Poster B2

Structural and electronic properties of epitaxial single-layer NbS$_2$ on Au(111) — •Raluca-Maria Stan, Sanjoy Mahatha, Charlotte Sanders, Davide Curcio, Marco Bianchi, Philip Hofmann, and Jill A. Miwa — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark

In this study, the epitaxial growth of single layer NbS$_2$ on a Au(111) substrate has been achieved and techniques like scanning tunneling microscopy, low-energy electron diffraction, and angle-resolved photoemission spectroscopy have been used in order to investigate its structural and electronic properties. The excellent crystalline quality is revealed by the well-ordered hexagonal moiré superstructure and a well-defined orientation with respect to the Au(111) substrate. An accurate determination of the hexagonal lattice constant indicates agreement with the lattice parameter of the bulk parent compound. The electronic structure reveals two electron pockets crossing the Fermi level with appreciable broadening that can be due to hybridization with the substrate or strong many-body effects in the system. The metallic character has been shown and the general shape of the band structure is consistent with the 1H configuration. No indication of a charge density wave formation has been observed at a temperature down to 30 K.

O 66.5 Wed 17:45 Poster B2

Characterisation of MoS$_2$ and WS$_2$ demonstrating a general approach for the synthesis of two-dimensional binary compounds — •Ann Julie Holt[1], Raluca Maria Stan[1], Marco Bianchi[1], Abhay Shivayogimath[2], Philip Hofmann[1], and Timothy Booth[2] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark — [2]DTU Nanotech, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

The synthesis of many two-dimensional materials is now scalable through different chemical vapor deposition (CVD) techniques. However, the crystal quality resulting from these methods is very sensitive to growth parameters and the details of the procedure are highly material-dependent. A significant amount of effort needs to be invested for the synthesis of each individual material, and the development of a general growth method would therefore be of great interest.

Here, we present an experimental study of two-dimensional single layer MoS$_2$ and WS$_2$ obtained from a general synthesis method developed for two-dimensional binary compounds. Structural and electronic characterization is performed by scanning tunneling microscopy (STM), low energy electron diffraction (LEED), and angle-resolved photoelectron spectroscopy (ARPES), showing high quality single-layer growth. These results serve as a proof of principle of a simple strategy for growing atomically thin binary compounds, which may greatly simplify the fabrication of already established and future two dimensional materials.

O 66.6 Wed 17:45 Poster B2

Growth and characterization of single layer tantalum phosphide compounds — •Federico Andreatta, Ann Julie U. Holt, Marco Bianchi, Jill A. Miwa, and Philip Hofmann — Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

Bulk transition metal pnictides have been recently found to host Weyl fermions, a novel state of topological quantum matter[1]. Transition metal pnictides are comprised of a transition metal and a group V element. Here, we show a method for growing tantalum phosphide compounds at the 2D limit on a Au(111) substrate. Using a combination of scanning tunneling microscopy and x-ray photoelectron spectroscopy we find two potential phases of single layer tantalum phosphide compounds. Intriguingly, one of the by-products of this growth method is single layer blue phosphorus[2]. We perform a systematic study of the growth parameters to tune the synthesis so that only single layer tantalum phosphide compounds are found at the surface.

[1] Z. K. Liu et al. Nat. Mater. (2015) 15, 27. [2] J. L. Zhang et al.

Nano Lett. (2016) 16, 4903.

O 66.7 Wed 17:45 Poster B2

A Two-dimensional Sub-stoichiometric Molybdenum Sulfide with Catalytically Active Basal Planes — Yang Bao[1,2], Ming Yang[3], and •Kianping Loh[1] — [1]Department of Chemistry, National University of Singapore, 117543 Singapore — [2]TUM Fakultät für Physik, James-Franck-Straße 1, 85748 Garching bei München — [3]Institute of Materials Research and Engineering, 117602, Singapore

2D molybdenum disulfide (MoS2) has attracted immense interests recently due to its remarkable optoelectronic and catalytic properties. Other than the thermodynamically stable MoS2 structure, different metastable, sub-stoichiometric phases of MoSx (x<2) may exist due to the versatile Mo-S coordination, which may offer unique functionalities not seen in MoS2. While 0D [Mo3S13]2- cluster (Kibsgaards et al. Nat Chem 6, 248-253, 2014) and 1D Mo6S6 wire (Lin et al. Nat Nano 9, 436-442, 2014) have been reported, 2D phases of MoSx compounds are less well studied. Under-coordinated atoms in such 2D Mo-S polymorphs may give rise to periodic spin textures or chemically reactive surface sites.

Here we report the discovery of a 2D sub-stoichiometric MoSx (x<2) phase, where interesting structural features such as undercoordinated surface sites were clearly revealed by surface characterization techniques. Density function theory (DFT) studies suggest that 2D-MoSx may have a Mo18S18 unit cell. We have carried out catalytic studies on its basal plane and observed its ability to catalyze oligomerization of molecules as well as the activation of molecular hydrogen into atomic hydrogen.

O 66.8 Wed 17:45 Poster B2

Hematene for the oxygen evolution reaction — •Yidan Wei, Mahdi Ghorbani-Asl, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz Zentrum Dresden Rossendorf, Dresden 01328, Germany

Using density functional theory (DFT) calculations, the catalytic activity of a recent member of two-dimensional (2D) materials, hematene (α-Fe2O3 monolayer), has been studied for oxygen evolution reactions (OER). The stability and electronic structure of two experimentally faceted sheets of hematene, (001) and (010), was investigated. It was found that the (001) facet (1.589 eV) exhibits lower cleaving energy in comparison to the (010) facet (1.892 eV) suggesting a more stable structure. The electronic structure calculations indicate that facets of hematene for (001) and (010) are semiconducting monolayer with a large energy gap of about 1.51 eV and 1.36 eV in comparison to its bulk counterpart (1.8-2.2 eV). We also studied the relationship between the experimentally observed facets and their OER catalytic reactivity. It is found that the determining step in the OER process is the reaction of a H2O molecule in the surface to form an adsorbed hydroxyl group (O*). The variation of Gibbs energy is around 0.4 eV at most. The (010) facet showed a lower barrier for oxygen evolution than (001) facet. It was also demonstrated that the adsorption free energy and onset overpotential can be further tuned by defects, such as vacancies.

O 66.9 Wed 17:45 Poster B2

Oxygen interaction with h-BN on Ni(111) — •Christian Papp[1], Florian Späth[1], Soni Himadri[2], Fabian Düll[1], Johann Steinhauer[1], Udo Bauer[1], Philipp Bachmann[1], Hans-Peter Steinrück[1], and Andreas Görling[2] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen — [2]Friedrich-Alexander Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Chemie , Egerlandstr. 3, 91058 Erlangen

Hexagonal boron nitride (h-BN) is an interesting material to study, as an isoelectronic and structural analogue to graphene. However, due to the ionic character of the boron-nitrogen bond a bandgap of ~5.4 eV is found. This makes h-BN an interesting dielectric for graphene-based 2D-transistors. Moreover the band gap is ideal for emission of UV-light. To further modify the properties of 2D materials a chemical functionalization is needed.

In an activated adsorption process, molecular oxygen forms a molecularly bound species on a supported h-BN layer on Ni(111) at room temperature. By increasing the sample temperature to 400 K, oxygen can be intercalated under h-BN. At 600 K and higher, even the oxidation of h-BN becomes possible. The system was studied by XPS and NEXAFS. The results are supported by DFT calculations.

O 66.10 Wed 17:45 Poster B2

Layer dependent properties of quasi-freestanding 2H-TaS$_2$ investigated with STM and STS — •Camiel van Efferen[1], Joshua Hall[1], Clifford Murray[1], Matthias Rolf[1], Niels Ehlen[1], Jun Li[1], Jan Berges[2], Erik van Loon[2], Tim Wehling[2], Alexander Grüneis[1], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Theoretische Physik, Bremen Center for Computational Materials Science, Universität Bremen, Germany

We epitaxially grow quasi-freestanding TaS$_2$ multilayers on graphene on Ir(111) and investigate their thickness dependent properties up to three layers.

Using scanning tunnelling microscopy we observe the monolayer to be in the expected 3×3 charge density wave (CDW) phase, whereas the bilayer unexpectedly shows a 2×2 superstructure. Furthermore, the moiré of Gr on Ir(111) is no longer visible through the bilayer. Due to finite bilayer island sizes confinement effects occur, which interact with the superstructure.

We probe the electronic structure with low temperature scanning tunnelling spectroscopy, and find a strongly decreased density of states around the Fermi energy, as would be expected for a CDW. The width of the gap is compared with its monolayer analogue. We disentangle contributions from intrinsic bilayer properties, stacking effects and local confinement effects to the electronic structure.

O 66.11 Wed 17:45 Poster B2

Revealing the hydrogenated structure of silicene r13xr13 by STM tip induced dehydrogenation — •jinglan qiu — Hebei Normal University, Shijiazhuang, China

Although ordered and reversible hydrogenation has been demonstrated on silicene 4x4 and 2r3x2r3 superstructures, the hydrogenated structure of silicene r13xr13 (type I and type II) have not yet been revealed. Recently, we find that atomic hydrogen desorption processes can be induced by field-emitted or tunneling electrons from the STM tip, converting the hydrogen terminated silicene to intact monolayer silicene, including 4x4, 2r3x2r3 and r13xr13 phases. Bombardment of the surface with low energy (above 3eV) electrons desorbs the hydrogen and creates a bias dependent desorption area under the tip apex. From the high resolution STM images before and after hydrogen desorption, we get the one-to-one correspondence between hydrogenated silicene and various silicene phases. Interestingly, for silicene r13xr13 (type I), the hydrogenated structure appears almost identical to half-silicane that formed on silicene 2r3x2r3, indicating it an intact monolayer silicene as well. However, the hydrogenated structure of silicene r13xr13 (type II) shows quite differently with small pieces of silicene 1x1 surrounded by various size of black holes that expose the Ag(111) substrate. Thus, silicene r13xr13 (type II) should be regarded as a "precursor phase" for more ordered phases such as 4x4 and r13xr13.

O 66.12 Wed 17:45 Poster B2

The surface of high-temperature non-IPR fullerides — Jürgen Weippert[1], Seyithan Ulas[1], Eugen Wald[1], Bastian Kern[1], Dmitry Strelnikov[1], Mateo Amatti[2], Luca Gregoratti[2], Maya Kiskinova[2], and •Artur Böttcher[2] — [1]Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — [2]Elettra, Sincrotrone Trieste, ScPA Area Science Park, 34149 Basovizza-Trieste, Italy

Alkali metal doped non-IPR fullerene materials C$_n$, ($n = 60 - 2k$ and $n = 70 - 2k$, $k = 1, ..5$) represent a new class of fullerides.[1] We created Cs$_x$C$_{58}$ and Cs$_x$C$_{68}$ materials making use of the low energy cluster beam deposition (LECBD [2]). The non-IPR fullerene cages C$_{58}$ and C$_{68}$ form a covalently stabilized scaffold which gets doped by Cs atoms already during the growth. By heating the resulting material up to 1100K monodispersed high-temperature carbon solids, HT-Cs$_x$C$_n$, can be created. The resulting materials exhibit high stability and considerably depleted Cs contents. The carbon scaffolds are stabilized by multifold covalent intercage bonds.[3] The surface morphology is driven by on-top segregation in the two-component system. In both HT materials the surface topography is dominated by islands standing out by their elevated Cs/C$_n$ ratio r.[1] Whereas the islands seen in Cs$_x$C$_{58}$ exhibit r values not larger than 2 the bright surface areas in the Cs$_x$C$_{68}$ solids surprise with extremely high r values (up to 70 Cs atoms per cage). [1] S. Ulas, et al. Phys. Status Solidi B 2018, 1800453 (1-13).[2] S. Ulas, et al. Carbon 2014, 68, 125-137.[3] S. Ulas, et al. J. Chem. Phys. 2012, 136, 114708.

O 66.13 Wed 17:45 Poster B2

Hydrogenation of bilayer graphene with excited H$_2$ — •Claus

F. P. Kastorp[1], Anders L. Jørgensen[2], Martha Scheffler[1], John D. Thrower[1], David A. Duncan[3], Tien-Lin Lee[3], Liv Hornekaer[1], and Richard Balog[1] — [1]Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — [2]The Mads Clausen Institute, SDU NanoSYD, Sønderborg, Denmark — [3]Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, United Kingdom

Hydrogenation of single graphene layers provides a pathway for band gap tuning [1], while in bilayer graphene, functionalization could result in the formation of a diamane [2]. STM measurements show that bilayer islands grown by CVD on Ir(111) are not functionalized by excited H_2, but single layer areas are [3]. Similarly, no hydrogenation is expected for full bilayer graphene samples produced via MBE on Ir(111).

I will present standard XPS and hard X-ray standing wave photoemission experiments that show a high degree of hydrogenation in MBE grown bilayer graphene when exposed to excited H_2 molecules. Specifically, the components of the photoemission spectra that are associated with the bottom graphene layer, which is in direct contact with the iridium surface, indicate a level of hydrogenation that is comparable to the hydrogenation found for single layer graphene when exposed to excite H_2. The top layer component appears mostly unaffected.

[1] Balog, et al. Nature materials 9.4 (2010): 315.
[2] Leenaerts, et.al., Phys. Rev. B, 80.24 (2009): 245422.
[3] Hansen, L.K., Ph.D. thesis, Aarhus University (2017).

O 66.14 Wed 17:45 Poster B2

Sample preparation for Graphene Enhanced Raman Spectroscopy — •Stephan Sleziona, Simon Rauls, Leonard Christen, Tobias Foller und Marika Schleberger — Universität Duisburg-Essen, AG Schleberger, Germany

Graphene-enhanced Raman spectroscopy (GERS) has been shown to be a powerful tool for ultrasensitive detection of adsorbed molecules [1]. As a possible mechanism charge transfer is often suggested, which depends on the Fermi-level of the graphene, the HOMO-LUMO levels of the molecules and the excitation laser energy [2, 3]. Therefore, a combination of changing the fermi level in a graphene-based field effect device (GFET) and the excitation laser energy allows to investigate the coupling of this hybrid system. We prepared GFETs in two different ways: (i) with graphene grown by chemical vapor deposition (CVD) using photolithography and (ii) with exfoliated graphene using electron beam lithography (EBL). Cobalt Octaethylporphyrin (CoOEP) is deposited via thermal evaporation onto our substrates and the growth is analyzed using Raman spectroscopy and atomic force microscopy. Furthermore, we compare these fully processed samples with pristine samples to study possible influences of our lithography process on the various properties, such as graphene quality, molecular adsorption, and changes in the charge transfer mechanism of GERS.

[1] X. Ling et al., Small, 6 (2010), pp. 2020*2025
[2] E.B. Barros et al., Phys. Rev. B, 90 (2014), 035443
[3] Q. Hao et al., Appl. Phys. Lett., 102 (2013), 011102