

O 47: 2D Materials II: Growth, Structure and Substrate Interaction I

Time: Wednesday 10:30–13:00

Location: GER 37

O 47.1 Wed 10:30 GER 37

Two-Dimensional Non-van der Waals Materials from Data-Driven Research — TOM BARNOWSKY^{1,2}, MAHDI GHORBANI-ASL¹, STEFANO CURTAROLO³, ARKADY V. KRASHENINNIKOV^{1,4}, and ●RICO FRIEDRICH^{1,2,3} — ¹Helmholtz-Zentrum Dresden-Rossendorf, Dresden — ²TU Dresden — ³Duke University, Durham, USA — ⁴Aalto University, Aalto, Finland

While two-dimensional (2D) materials are traditionally derived from bulk layered compounds bonded by weak van der Waals (vdW) forces, the recent surprising experimental realization of non-vdW 2D compounds obtained from non-layered crystals [1] foreshadows a new direction in 2D systems research.

Here, we present several dozens of candidates of this novel materials class derived from applying data-driven research methodologies in conjunction with autonomous *ab initio* calculations [2,3]. We find that the oxidation state of the surface cations of the 2D sheets is an enabling descriptor regarding the manufacturing of these systems as it determines their exfoliation energy: small oxidation states promote easy peel off [2]. When extending the set from oxides to sulfides and chlorides, the exfoliation energy becomes ultra low due to strong surface relaxations [3]. The candidates exhibit a wide range of appealing electronic, optical and magnetic properties making these systems an attractive platform for fundamental and applied nanoscience.

[1] A. Puthirath Balan *et al.*, Nat. Nanotechnol. **13**, 602 (2018).

[2] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).

[3] T. Barnowsky *et al.*, submitted (2022).

O 47.2 Wed 10:45 GER 37

Phase Transitions of the BlueP-Au-network on Au(111) by Intercalation of Potassium — PHILIP GRIMM, ●FELIX OTTO, MAXIMILIAN SCHAAL, FLORENTINE FRIEDRICH, ROMAN FORKER, and TORSTEN FRITZ — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

In 2014, a new elemental semiconductor was postulated: Blue Phosphorene (BlueP). This monolayer of P atoms offers a layer thickness-dependent band gap and high charge carrier mobility. However, the synthesis of a highly ordered and stable monolayer of BlueP is still a challenge and could only be achieved on gold substrates by constructing a Au-P network. This undesirable coupling, which leads to a change in electronic properties, could be mitigated by the intercalation of potassium. The goal is to synthesize a free-standing monolayer of BlueP. The effects of substrate temperature during K deposition and the order of deposition of phosphorus and potassium on Au(111) were investigated. Structural properties were characterized by LEED and RHEED, chemical properties by XPS, and electronic properties by photoelectron spectroscopy methods ((AR)UPS and PMM). In the end, a (2×2) superstructure is obtained. This superstructure exhibited the most promising electronic properties, which were very close to those of the free-standing BlueP. It is assumed that K and P together form the basis of the (2×2) superstructure, since the reactive bonds of potassium could be saturated and stabilized by phosphorus. At temperatures of 250 °C, the BlueP-Au network dissolves under the influence of potassium deposition and various intermediates are formed.

O 47.3 Wed 11:00 GER 37

Structural and chemical characterization of epitaxially grown FeBr₂ on Au(111) — ●S. E. HADJADJ¹, C. GONZALEZ-ORELLANA², J. LAWRENCE³, D. BIKALJEVIC^{4,5}, M. PENA-DIAZ², P. GARGIANI⁶, L. ABALLE⁶, J. NAUMANN⁷, M. A. NINO⁶, M. FOERSTER⁶, S. RUIZ-GOMEZ⁸, S. THAKUR¹, I. KUMBERG¹, J. TAYLOR⁹, J. HAYES¹, J. TORRES¹, C. LUO⁹, F. RADU⁹, D. G. DE OTEYZA³, W. KUCH¹, J. I. PASCUAL⁴, C. ROGERO^{2,3}, and M. ILYN² — ¹Freie Universität Berlin, Institut für Experimentalphysik, Germany — ²Centro de Física de Materiales, Donostia, Spain — ³Donostia International Physics Center, Spain — ⁴CIC nanoGUNE-BRTA, Donostia, Spain — ⁵Institute of Physical Chemistry, University of Innsbruck, Austria — ⁶ALBA Synchrotron Light Source, Spain — ⁷Freie Universität Berlin, Dahlem Center for Complex Quantum Systems, Germany — ⁸Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — ⁹Helmholtz-Zentrum Berlin, Germany

We present structural, chemical and magnetic properties of the van der Waals material FeBr₂ on Au(111) with thicknesses from submono-

layer to multilayer. We observe that the first layer on Au(111) shows a dominant superstructure. The chemical characterization by XPS and XAS shows that the material is growing in the same composition for different thicknesses. The magnetic characterization by XMCD reveals that the magnetic moment increases with increasing thickness.

O 47.4 Wed 11:15 GER 37

Formation of Europium transition metal surface compounds and its protection below hBN — ●ALAA MOHAMMED IDRIS BAKHIT^{1,2}, KHADIZA ALI^{3,4}, ANNA A. MAKAROVA^{4,5}, IGOR PIŠ⁶, FEDERICA BONDINO⁶, and FREDERIK SCHILLER^{1,4} — ¹MPC, San Sebastián, Spain — ²Universidad del País Vasco, San Sebastián, Spain — ³Chalmers University of Technology, Göteborg, Sweden — ⁴DIPC, San Sebastián, Spain — ⁵FU Berlin, Germany — ⁶IOM-CNR, Trieste, Italy

We present a comparative study of the electronic and structural properties of hBN on curved transition metal (TM) substrates, namely, Ni, Rh and Pt crystals and their modifications after Eu intercalation. hBN was grown by CVD processes. The growth quality depends strongly on the lattice mismatch and the overlayer-substrate interaction. The interface properties could be influenced by tuning the substrate material and its step density. That was shown by hBN growth on curved crystals that feature strong (Ni), medium (Rh) or weak (Pt) substrate interaction. The structural properties were investigated by Low-energy electron diffraction (LEED) and scanning tunnelling microscopy (STM). Stable facets are formed upon hBN growth on the substrates, which are changed after Eu intercalation. A formation of Eu-TM alloy is detected. The electronic structure was characterized by X-ray photoelectron spectroscopy (XPS) and angle-resolved photoemission measurements (ARPES). We studied the possible protection of Eu by the hBN layer. We observe that Eu protection was incomplete due to defects and hBN growth boundaries which resulted in Eu oxidation.

O 47.5 Wed 11:30 GER 37

Interaction of Au and Rh metals with h-BN on Rh(111) from theoretical calculations — ●KRISZTIÁN PALOTÁS — Wigner Research Center for Physics, Budapest, Hungary — ELKH-SZTE Reaction Kinetics and Surface Chemistry Research Group, Szeged, Hungary

Based on density functional theory calculations, the interaction of Au and Rh metal deposits with hexagonal boron nitride (h-BN) monolayer on a Rh(111) substrate in different model systems is studied. Significant differences in the metals' adsorption, growth and intercalation mechanisms are identified [1]. As an example, the formation of a 19-atoms Rh island in the pore of the nanomesh exhibits 3D growth, in contrast to a 2D island formation of Au [2]. We found that nitrogen vacancies and Rh show systematically lower energy barrier for atomic intercalation than boron vacancies and Au. Intercalation through the middle of a BN-divacancy provided the smallest energy barriers in our considered model systems. Our theoretical results provide a microscopic understanding of related experimental results [1].

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[1] G. Vári *et al.* submitted (2022). [2] A. P. Farkas *et al.* Appl. Catal. A Gen. **592**, 117440 (2020).

O 47.6 Wed 11:45 GER 37

Local Electronic Structure of h-BN on Pt(110) — ●MARCO THALER¹, FLORIAN MITTENDORFER², ERMINALD BERTEL¹, and LAERTE PATERA¹ — ¹Institute of Physical Chemistry, University of Innsbruck, Austria — ²Institute of Applied Physics and Center for Computational Materials Science, Vienna University of Technology, Austria

The growth of large-scale single-orientation hexagonal boron nitride (h-BN) monolayer has been recently achieved on the Pt(110) surface, exploiting the inversion of the normal substrate-adsorbate relation [1]. Here we performed Scanning Tunneling Spectroscopy to locally probe the electronic structure of h-BN and investigate the bonding configuration in detail. The moiré pattern arising from the mismatch with the substrate is observed to induce a modulation of the conduction

band onset of h-BN and a shift of the Pt-related state, implying varying interaction energies. In agreement with density functional theory, the local density of states near the Fermi energy indicates a localized covalent bonding between h-BN and Pt, causing a (1 \times n)-missing row reconstruction of the Pt(110) surface. [1] D. Steiner, et al., ACS Nano, 13, 7083-7090 (2019).

O 47.7 Wed 12:00 GER 37

Chemical vapor deposition of high optical quality large area monolayer Janus transition metal dichalcogenides — ●A. GEORGE¹, Z. GAN¹, I. PARADISANOS², A. ESTRADA-REAL², J. PICKER¹, E. NAJAFIDEHAGHANI¹, F. DAVIES³, C. NEUMANN¹, C. ROBERT², K. WATANABE⁴, T. TANIGUCHI⁴, X. MARIE², J. BISKUPEK⁵, M. MUNDZINGER⁵, R. LEITER⁵, U. KAISER⁵, A. KRASHENINNIKOV³, B. URBASZEK², and A. TURCHANIN¹ — ¹Friedrich Schiller University Jena, Jena, Germany — ²Université de Toulouse, Toulouse, France — ³Helmholtz-Centre Dresden Rossendorf, Dresden, Germany — ⁴National Institute for Materials Science, Tsukuba, Japan — ⁵University of Ulm, Ulm, Germany

Large scale chemical vapor deposition growth of Janus SeMoS monolayers is reported, with the asymmetric top (Se) and bottom (S) chalcogen atomic planes with respect to the central transition metal (Mo) atoms. The formation of these 2D semiconductor monolayers takes place upon the thermodynamically driven exchange of the bottom Se atoms of the initially grown MoSe₂ single crystals on gold foils with S atoms. The growth process is characterized by complementary experimental techniques including Raman and X-ray photoelectron spectroscopy, transmission electron microscopy, and the growth mechanisms are rationalized by first-principles calculations. The remarkably high optical quality of the synthesized Janus monolayers is demonstrated by optical and magneto-optical measurements which reveal the strong exciton-phonon coupling and enable to obtain an exciton g-factor of -3.3. (Adv. Mater. 34, 2022, 2205226)

O 47.8 Wed 12:15 GER 37

Preparation and characterization of carborane based nanomembranes — ●MARTHA FREY¹, JULIAN PICKER¹, JAKUB VIŠŇÁK², CHRISTOF NEUMANN¹, TOMÁŠ BAŠE², and ANDREY TURCHANIN¹ — ¹Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — ²The Czech Academy of Sciences, Institute of Inorganic Chemistry, 250 68 Husinec-Rez, c.p. 1001, Czech Republic

Carboranes are electron-delocalized molecular clusters containing boron, carbon, and hydrogen. Because of their high chemical and thermal stability as well as their structural variability, they are interesting for a wide range of applications including nanoscale engineering, catalysis, and boron neutron capture therapy. Here, we present the fabrication of a novel boron-based two-dimensional (2D) material *via* electron irradiation induced cross-linking of carborane self-assembled monolayers (SAMs) on silver substrates. Using the double-cage molecule 1,2-dicarba-*closo*-dodecaborane-9,12-dithiol, the fabrication of a mechanically stable and continuous ~1 nm thin membrane was achieved. The self-assembly, cross-linking and transfer of the resulting nanomembranes onto grids have been characterized with different complementary surface-sensitive techniques including X-ray photoelectron spec-

troscopy (XPS), low-energy electron diffraction (LEED), ultraviolet photoelectron spectroscopy (UPS) and scanning electron microscopy (SEM).

O 47.9 Wed 12:30 GER 37

A Metastable Pentagonal 2D Material Synthesized by Symmetry-Driven Epitaxy — ●LINA LIU^{1,2} and YONG CHEN^{1,2} — ¹Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana, 47907, USA — ²Institute of Physics and Astronomy and Villum Centers for Dirac Materials and for Hybrid Quantum Materials and Devices, Aarhus University, 8000 Aarhus-C, Denmark

Most two-dimensional (2D) materials experimentally studied so far have hexagons as their building blocks. Only a few exceptions, such as PdSe₂, are lower in energy in pentagonal phases and exhibit pentagons as the building blocks. Such pentagonal 2D materials demonstrate unprecedented properties and unique applications originated from low-symmetry lattice geometries. While theory has predicted a large number of pentagonal 2D materials, many of them are metastable and their experimental realization is difficult. Here, we report the first synthesis of a metastable pentagonal 2D material, the pentagonal PdTe₂ monolayer, by symmetry-driven epitaxy. Scanning tunneling microscopy is used to characterize the monolayer pentagonal PdTe₂, which demonstrates well-ordered low-symmetry atomic arrangements. Theoretical calculations, along with angle-resolved photoemission spectroscopy, reveal the band structures of monolayer pentagonal PdTe₂. In contrast to the narrow bandgap of monolayer hexagonal PdTe₂, monolayer pentagonal PdTe₂ is a semiconductor with a much bigger indirect bandgap of 1.08 eV. Our work opens an avenue for the synthesis of new, pentagon-based 2D materials and gives great opportunities to explore their applications such as multifunctional electronics.

O 47.10 Wed 12:45 GER 37

The transformation of 2D honeycombs into dodecagonal quasicrystals — ●STEFAN FÖRSTER, LOI VINH TRAN, MARTIN HALLER, SEBASTIAN SCHENK, and WOLF WIDDRA — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Oxide quasicrystals are 2D materials with an aperiodic dodecagonal symmetry [1]. Starting from a binary oxide Ti₂O₃ honeycomb structure on Pt(111), the Ti_nO_n ring structure with n=6 is transformed into a network of rings with ring sizes of n= 4, 5, 7 and 10 in the presence of Ba atoms. In these networks, n=7 rings host one Ba atom and n=10 rings host two [23].

In this contribution, the basic mechanisms for the network transformation are discussed. Stone-Wales transformations are the key mechanism to realize n=4...7 rings. In addition, by incorporating an additional oxygen atom, two neighboring n=6 rings convert into a n=10 ring [3]. The amount of Ba controls this conversion process and leads to a sequence of long-range ordered structures including a well-defined quasicrystal.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, Nature **502**, 215 (2013)

[2] E. Cockayne et. al, Phys. Rev. B **93**, 020101(R) (2016)

[3] S. Schenk, O. Krahn, E. Cockayne, H. L. Meyerheim, M. De-Boissieu, S. Förster, and W. Widdra, Nat. Commun, accepted (2022)