O 72: 2D Materials beyond graphene: Growth, structure and substrate interaction – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

O 72.1 Wed 18:00 P2

In-Situ CVD growth of vertical Heterostructures of Borophene and Hexagonal Boron Nitride — •Niels Ganser[1], Marko Kriegel[1], Smruti Ranjan Mohanty[1], Karim Omambac[1], Marin Petrovic[2], Christian Brand[1], Steffen Franzka[3], Birk Finke[1], Tobias Hartl[4], Thomas Michely[4], Frank-Joachim Meyer zu Heringdorf[1,3], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen — [2]Institute of Physics, Zagreb — [3]ICAN, Duisburg — [4]Universität zu Köln

Intrinsic segregation provides a promising and scalable route for the in situ fabrication of 2D heterostructures. Using UHV chemical vapor deposition (CVD) of a single borazine ($B_3N_3H_6$) precursor [1], we demonstrate the growth of an hBN/borophene heterostructure on Ir(111). At high temperatures and low precursor pressures, boron dissolves into the Ir subsurface region, creating a boron reservoir below the surface [2]. Largely increasing the precursor dosing pressure shifts the chemical potential toward the formation of a complete hBN layer. Upon cooldown, the decreasing boron solubility of the Ir substrate drives segregation to the surface, where a borophene layer forms underneath the hBN overlayer and thus completing the heterostructure. The resulting structure and its growth kinetics were investigated using a combined low energy electron diffraction (SPA-LEED) and microscopy (LEEM) approach.

[1] K. Omambac et al., ACS Nano 17 (2023) 17946

[2] K. Omambac et al., ACS Nano 15 (2021) 7421

O 72.2 Wed 18:00 P2

Growth of 2D molecular networks on graphene — •Haruto Shibahara and Toyo Kazu Yamada — Dept. Materials Science, Chiba Univ., Chiba, Japan

We demonstrate the engineering of qubits on solid surfaces using organic molecules and transition-metal magnetic atoms. Atomically flat and clean graphene (Gr) grown on an Ir(111) substrate was selected as the platform. Scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) revealed the characteristic moiré pattern, while scanning tunneling spectroscopy (STS) and angle-resolved photoemission spectroscopy (ARPES) confirmed the presence of Dirac bands. Although single atoms can in principle serve as qubits, they tend to thermally diffuse on surfaces and their energy levels may remain degenerate. To overcome these issues, it is necessary to coordinate the atoms with organic ligands, whose ligand fields can lift the degeneracy. As a first approach, we attempted to employ 1,3,5-tris(4-bromophenyl)benzene (TBB) molecules to form a two-dimensional (2D) covalent organic framework. However, on the Gr surface we found that thermal activation desorbed the TBB molecules before they could undergo Ullmann coupling. As a second approach, we attempted to grow a 2D metal organic framework (MOF) on Gr. The details of this effort will be discussed.

O 72.3 Wed 18:00 P2

Probing the Electrostatic Potential of hBN by AFM with Oxygen-Terminated Copper Tips — •Jan ter Glane[1,2], Philipp Wiesener[1,2], Thorsten Deilmann[3], Milena Merkel[1,2], Maciej Bazarnik[2], Anika Schlenhoff[2], and Harry Mönig[1,2] — [1]Center for Nanotechnology, University of Münster, Germany — [2]Institute of Physics, University of Münster, Germany — [3]Institute of Solid State Theory, University of Münster, Germany

Monolayer hexagonal boron nitride (hBN) hosts point defects with promising optoelectronic properties, yet their atomic structure remains unclear [1]. Conventional scanning tunneling (STM) and atomic force microscopy (AFM) lack elemental contrast, making it difficult to reliably distinguish B and N sites. Non-contact AFM with oxygen-terminated copper tips (CuOx-tips) has previously enabled elemental discrimination and defect identification on metal oxides [2].

Using CuOx-tip AFM, we demonstrate elemental contrast on NaCl thin films, suggesting its broad applicability to polarized surfaces. Leveraging this capability, we investigate its application to monolayer hBN. DFT-optimized electrostatic potential calculations predict clear B-N contrast. To realize these measurements, we employ in-situ chemical vapor deposition growth procedures for high-quality hBN on single-crystalline substrates. We outline the benefits of CuOx-tip AFM and present initial results towards correlating STM/STS measurements, aiming to enable atom-specific defect identification in hBN.

[1] Grosso *et al.*, Nat. Commun. **8**, 705 (2017)

[2] Wiesener *et al.*, ACS Nano **18**, 21948 (2024)

O 72.4 Wed 18:00 P2

Pt-doped borane nanomembranes — •Martha Frey[1], Julian Picker[1], Christof Neuman[1], Jan Macháček[2], Tomáš Base[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — [2]The Czech Academy of Sciences, Institute of Inorganic Chemistry, 250 68 Husinec Rez, 1001, Czech Republic

Boranes are clusters of boron and hydrogen atoms that form three-dimensional, cage-like molecules. We have recently employed them as convenient starting precursors for synthesising two-dimensional (2D) carbon-free nanomembranes. In this study, we present the preparation and characterisation of the self-assembled monolayers (SAMs) of two thiolated *syn*-$B_{18}H_{22}$ clusters on silver substrates. Subsequently, these SAMs were cross-linked laterally to form boron nanomembranes (BNMs) via low-energy electron irradiation under ultra-high vacuum (UHV) conditions. We investigated the structural and chemical properties of these 2D nanomembranes using surface-sensitive techniques such as X-ray photoelectron spectroscopy (XPS) and scanning tunnelling microscopy (STM). Both the starting SAMs and the resulting boron nanomembranes exhibited reactivity toward Pt-containing complexes. While such reactivity was expected for the SAMs, it was particularly noteworthy that the BNMs also enabled the insertion of Pt atoms. This Pt-doping positions borane-derived SAMs and BNMs as a promising 2D platform for nanoscale catalytic studies.

O 72.5 Wed 18:00 P2

Defects and Initial Approaches to TMDC Heterostructure Growth on $\mathbf{Pt_xTe_y}$ films — •Isabella Stollberg, Andreas Raabgrund, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Transition-metal dichalcogenides (TMDCs) can generally be synthesised either by co-evaporating the metal and chalcogen onto a suitable substrate [1] or by depositing only the chalcogen onto the desired metal surface. Using STM, STS, and DFT, we investigate Pt_xTe_y films on Pt(111) prepared via the latter approach. With increasing Te content, different initial growth surface telluride structures are observed, followed by the formation of Pt_2Te_2 and $PtTe_2$ layers [2]. This contribution focuses on STM and spatially resolved STS analyses of point defects in $PtTe_2$, as well as domain boundaries within a $PtTe_2$ or Pt_2Te_2 layer. Furthermore, we evaluate the suitability of these telluride films as substrates for TMDC heterostructure growth. First results on attempting to grow $TiTe_2$ and $PdTe_2$ demonstrate considerable intermixing. While $TiTe_2$ islands can be identified by their apparent height and other lattice constants, $PdTe_2$ islands cannot be distinguished from $PtTe_2$ based on topography due to their similar vertical and lateral lattice parameters.

[1] K. Lasek et al., Nano Lett. **22**, 23 (2022)

[2] T. Kißlinger et al., Phys. Rev. B **108**, 205412 (2023)

O 72.6 Wed 18:00 P2

Boosting the Efficiency of Quantum Replica-Exchange Molecular Dynamics — •Jan-Niklas Mohr, Shubham Sharma, and Mariana Rossi — MPI for the Structure and Dynamics of Matter, Hamburg, Germany

Replica exchange molecular dynamics can be combined with path-integral techniques in order to incorporate quantum statistics in the sampled ensembles [1]. However, the efficiency in swapping replicas is decreased to a point that makes simulations extremely inefficient at lower temperatures.

We propose a new acceptance criterion for path-integral replica-exchange molecular dynamics (PI-REMD) that incorporates the path-integral spring term in the Hamiltonian and rescales it consistently. As a result, the acceptance probability is only sensitive to potential-energy differences, and the efficiency of the method is thus increased. Benchmarking on several test systems, including asymmetric double wells and glassy-like potentials, shows that our method outperforms standard PI-REMD in sampling efficiency and exchange frequency. We also show improvements for realistic materials, such as monolayer 1H-TaS_2 [2], where it is paramount to obtain an accurate description of the charge-density-wave phase transition. Our acceptance criterion therefore provides an efficient and reliable tool for studying quantum phase transitions and exploring thermodynamic ensembles under challenging conditions.

[1] Kapil *et al.*, Comput. Phys. Commun. 236, 214-223 (2019).
[2] Schobert *et al.*, SciPost Phys. 16, 046 (2024)