

O 59: 2D Materials III: Nanomembranes, hBN, and Particle Interactions

Time: Wednesday 15:00–17:30

Location: H16

O 59.1 Wed 15:00 H16

Molecular dynamics investigation of Young's moduli of carbon nanomembranes (CNMs) — ●JULIAN EHRENS¹, FLORIAN GAYK¹, TJARK HEITMANN², PATRICK VORNDAMME¹, and JÜRGEN SCHNACK¹ — ¹Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany — ²Osnabrück University, Neuer Graben/Schloss, 49074 Osnabrück, Germany

Nanometer thin carbon nanomembranes (CNMs) are made by electron-induced crosslinking of aromatic self-assembled monolayers (SAMs) [1]. Their supposedly irregular internal structure can not be adequately investigated by X-ray diffraction, but by a characterization through physical quantities like solvent permeability and Young's modulus. In order to propose possible structures of these membranes we investigate various initial configurations of the SAM and excitation processes that mimic the impact of the radiation together with their impact on the Young's modulus. For all calculations classical molecular dynamics as implemented in LAMMPS is employed. Preliminary studies have been made in benchmarking the accuracy of several classical carbon potentials concerning Young's moduli [2]. We discuss two methods to obtain the moduli: application of homogeneous scaling and directional strain to the monolayer.

[1] Turchanin et al., *Progress in Surface Science*, Volume 87, Issues 5-8, May-August 2012, Pages 108-162

[2] Gayk et al., *Physica E: Low-dimensional Systems and Nanostructures*, Volume 99, May 2018, Pages 215-219

O 59.2 Wed 15:15 H16

Preparation of Carbon Nanomembranes from SAMs with carboxylic binding groups on silver substrates — ●CHRISTOP NEUMANN¹, MONIKA SZWED², MARTHA FREY¹, ZIAN TANG¹, PIOTR CYGANIK², and ANDREY TURCHANIN¹ — ¹Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — ²Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland

The electron irradiation induced synthesis of Carbon Nanomembranes (CNMs) from aromatic thiol-based self-assembled monolayers (SAM) is a well-established method to form molecular thin nanosheets [1]. These molecular 2D materials can be prepared with tunable properties and therefore they find a variety of applications in nanotechnology ranging from ultrafiltration to nanobiosensors [2]. Here we study the conversion of SAMs with aromatic-aliphatic backbones and carboxylic head groups [3,4] into CNMs on silver substrates. To this end, we employ high-resolution X-ray photoelectron spectroscopy, low-energy electron diffraction, atomic force microscopy and scanning electron microscopy. We find a clear correlation between the length of the aliphatic chain in the precursor molecules and the properties of the formed CNMs. Moreover, we compare these results with the formation of CNMs from thiol-based molecular counter partners. [1] P. Angelova, A. Turchanin et al., *ACS Nano* 7, 6489-6497 (2013) [2] A. Turchanin, A. Götzhäuser, *Adv. Mater.* 28, 6075-6103 (2016) [3] A. Krzykawska, P. Cyganik et al., *Chem. Comm.* 53,5748-5751 (2017) [4] A. Krzykawska, P. Cyganik et al., *J. Phys. Chem. C* 122, 919-928 (2018)

Invited Talk

O 59.3 Wed 15:30 H16

Carbon Nanomembranes: Preparation, Properties, and Applications — ●XIANGHUI ZHANG — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Carbon Nanomembranes (CNMs) are two-dimensional sheets with tailored physical and chemical properties. I will first give an overview of the preparation of CNMs and their mechanical, optical and electronic characteristics. Then I will present several recent findings on the structure of CNMs using surface-enhanced Raman spectroscopy and scanning probe microscopy, which make CNMs of interest for applications in energy storage and membrane separations. Finally, I will show the realization of all-carbon capacitors composed of CNMs as dielectrics sandwiched between two graphene electrodes, and will further address how the CNM allows for a fast yet selective transport of water and helium through sub-nanometer channels.

[1] A. Turchanin, A. Götzhäuser, *Adv. Mater.* 28, 6075 (2016) [2] X. Zhang, M. Mainka, et al., *Langmuir*, 34, 2692 (2018) [3] X. Zhang, E. Marschewski, et al., *ACS Nano*, 12, 10301 (2018) [4] Y. Yang, P. Dementyev, et al., *ACS Nano*, 2018, 12, 4695 (2018)

O 59.4 Wed 16:00 H16

Au-Rh surface alloy for tuning the nanomesh structure of h-BN — ●KRISZTIÁN PALOTÁS^{1,2,3}, LÁSZLÓ ÖVÁRI³, GÁBOR VÁRI³, RICHÁRD GUBÓ³, ARNOLD FARKAS³, JÁNOS KISS³, ANDRÁS BERKÓ³, and ZOLTÁN KÓNYA³ — ¹Wigner Research Center for Physics, Hungarian Academy of Sciences, Budapest, Hungary — ²Budapest University of Technology and Economics, Budapest, Hungary — ³University of Szeged, Szeged, Hungary

Hexagonal boron nitride (h-BN) monolayer on the Rh(111) substrate has a periodically corrugated "nanomesh" structure. On the other hand, h-BN layer on a clean Au(111) substrate is atomically flat. By forming surface alloys of Au-Rh in different compositions on a Rh(111) substrate, we report on the gradual tunability of the nanomesh morphology of h-BN [1], which can be useful for various nanopatterning applications. Increasing the Au amount in the surface alloy results in reduced pore diameter and corrugation of the h-BN layer [1]. The experimental findings are confirmed by density functional theory calculations: The energetically preferred ordered (2x1) Au-Rh surface alloy [2,3] is reconstructed, and Rh is accumulated below the pore of h-BN.

References: [1] R. Gubó et al., *Phys. Chem. Chem. Phys.* 20, 15473 (2018). [2] L. Óvári et al., *Phys. Chem. Chem. Phys.* 18, 25230 (2016). [3] K. Palotás et al., *J. Phys. Chem. C* 122, 22435 (2018).

O 59.5 Wed 16:15 H16

Real-time investigation of the growth of hexagonal boron nitride on the Ni(111) surface — ●MIRIAM RATHS^{1,2}, JANINA FELTER^{1,2}, and CHRISTIAN KUMPF^{1,2} — ¹Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — ²Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology, Germany

The 2D material hexagonal boron nitride (hBN) has attracted strongest interest recently due to its specific structural and electronic properties. In this study, we aim for a deeper understanding of its nucleation and growth behavior, as this is necessary to produce high quality layers of hBN.

The growth of hBN on the Ni(111) surface depends strongly on the preparation of the substrate before deposition. In our study, we have used two different cleaning methods for the substrate resulting in different defect densities. In both cases, the growth of hBN was imaged in-situ and in real time by means of LEEM. Four different structures were found on the surface: (1) A commensurate and (2) a rotated hBN monolayer structure, the latter with various azimuthal rotation angles, as well as two bilayer structures consisting of either (3) two rotated or (4) one commensurate and one rotated layer of hBN. While the formation of all of these structures was observed on the Ni(111) surface with low defect density, at higher defect density only the two monolayer phases were found. For both growth experiments, we present a detailed analysis of (bright and dark field) LEEM and μ LEED data.

O 59.6 Wed 16:30 H16

How Graphene and Hexagonal Boron Nitride Get Electrified in Water? — ●BENOIT GROSJEAN, MARIE-LAURE BOCQUET, and RODOLPHE VUILLEUMIER — PASTEUR, Département de chimie, École normale supérieure, PSL University, Sorbonne Université, CNRS, 75005, Paris, France

The recent emergence of nanofluidics has highlighted the exceptional properties of graphene and its boron-nitride counterpart (hBN) as confining materials for water and ion transport. Surprisingly ionic transport experiments have unveiled a large electrification of the water-BN surfaces, with a contrasting response for its water-carbon homologue. This charging was conjectured to originate in the differential hydroxide adsorption on the 2D materials, but the challenge of simulating this elusive anion has precluded a proper explanation up to now. We report free energy calculations based on ab initio molecular dynamics simulations of a hydroxide in water near graphene and hBN layers. Our results(1) disclose that both surfaces electrify by hydroxide adsorption via different mechanisms. OH⁻ shows strong chemisorption on hBN, but only weak physisorption on graphene. Interestingly OH⁻ is shown to keep a fast lateral interfacial mobility while physisorbed. Taking into account the resulting large ionic surface mobility, an analytical transport model allows to reproduce quantitatively the experimental

data. Our results offer new foundations for the chemical reactivity of carbon and BN materials in water and suggest new perspectives for advanced membrane technologies for water purification and energy harvesting.

(1) B. Grosjean, M.-L. Bocquet and R. Vuilleumier, Submitted, 2018

O 59.7 Wed 16:45 H16

Charge exchange between highly charged ions and 2D materials — ●SASCHA CREUTZBURG^{1,2}, JANINE SCHWESTKA³, MUKESH K. TRIPATHI⁴, HEENA INANI⁴, RENÉ HELLER¹, NICO KLINGNER¹, ANNA NIGGAS³, TIBOR LEHNERT⁵, ROBERT LEITER⁵, ROLAND KOZUBEK⁶, STEFAN FACSKO¹, UTE KAISER⁵, JANI KOTAKOSKI⁴, MARIKA SCHLEBERGER⁶, FRIEDRICH AUMAYR³, and RICHARD A. WILHELM^{1,3} — ¹Helmholtz-Zentrum Dresden-Rossendorf, Ion Beam Center, Dresden, Germany — ²TU Dresden, Germany — ³TU Wien, Institute of Applied Physics, Vienna, Austria — ⁴University Vienna, Faculty of Physics, Austria — ⁵Ulm University, Central Facility of Electron Microscopy, Ulm, Germany — ⁶University Duisburg-Essen, Faculty of Physics and CENIDE, Duisburg, Germany

The neutralisation of ions due to their interaction with matter deals with fundamental aspects of ion-solid interaction, e.g.: How does the kinetic energy loss depend on the charge exchange? In order to investigate the neutralisation behaviour, classical ion beam foil experiments were performed using ultimately thin 2D materials as target. Because of their low thickness, an ion with a sufficiently high incident charge state does not reach charge equilibrium, which enables the measurement of the non-equilibrium exit charge state distribution. The influence of target material properties on the charge exchange is investigated for 2D materials consisting of graphene, MoS₂ and hBN, which show different band gap energies between 0 and 6 eV, conductance properties (metallic, semi-conducting and insulating) and layer structures.

O 59.8 Wed 17:00 H16

Unraveling energy-loss processes of low energy heavy ions in 2D materials — ●RICHARD A. WILHELM^{1,2} and PEDRO L. GRANDE³ — ¹TU Wien, Institute of Applied Physics, Austria — ²HZDR, Institute of Ion Beam Physics and Materials Research, Germany — ³Federal University of Rio Grande do Sul, Institute of Physics, Ion Implantation Laboratory, Brazil

In order to use ion beams for defect engineering of 2D materials, a model for energy deposition is needed, which takes the ion charge state and charge exchange into account. In the first monolayers of a mate-

rial impinging keV ions capture electrons and reduce their charge state until charge equilibrium is reached in less than 10 fs (about 1 nm).

We present here a new model for charge state and charge exchange dependent ion stopping force calculation, which shows that heavy ions in charge states greater than 1 deposit a substantially larger amount of their kinetic energy in a 2D material than predicted by standard tools as e.g. SRIM. This holds true for electronic and nuclear energy losses, whereas especially the latter causes sputtering and therefore structural defects.

Our model relies on a time-dependent scattering potential, which changes due to charge exchange and electronic de-excitation of the projectile during collision. We compare our model results with experimental values determined by heavy highly charged ion transmission through freestanding single layer graphene and find very good agreement in energy loss, charge state distributions, and scattering angle-dependent charge exchange.

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Characterization of interlayer forces in 2D heterostructures using neutral atom scattering — ●AMJAD AL TALEB^{1,2}, GLORIA ANEMONE¹, RODOLFO MIRANDA^{1,2,3,4}, and DANIEL FARIÁS^{1,3,4} — ¹Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain — ²Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nanociencia), Madrid, Spain — ³Instituto ‘Nicolás Cabrera’, Madrid, Spain — ⁴Condensed Matter Physics Center (IFIMAC), Madrid, Spain

We show that neutral atom scattering is suitable to determine the coupling strength between a two-dimensional (2D) material and the underlying substrate. This information can be obtained from the thermal attenuation of the specular intensity, as well as from angular distributions of He and Ne atoms in the low incident energy (20-50 meV) regime. For graphene (Gr) grown on several metal substrates, there is a direct correlation between the slope of thermal attenuation measurements and the Gr-substrate coupling strength obtained from surface phonons measurements. In addition, Ne scattering presents a broad, classical angular distribution when the Gr-substrate coupling is weak, like in Gr/Ir(111), whereas sharp diffraction features are observed for strongly interacting systems, like Gr/Ru(0001). The influence of the moiré superstructures on this simple picture is also discussed. This superstructures induces a splitting of the flexural mode of Gr in addition of additional phonon dispersion lines as a result of Umklapp scattering. We show evidence of the localization of the phonon modes from the difference in their thermal attenuation behaviors.