O 93: Poster Session VII: Graphene and beyond I

Time: Thursday 10:30–12:30 Location: P

O 93.1 Thu 10:30 P

Electric-field control of a single-atom polar bond — •Maryam Omidian[1], Susanne Leitherer[2], Nicolas Néel[1], Mads Brandbyge[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [2]Center of Nanostructured Graphene, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The polar chemical bond between a single Au atom terminating the apex of an atomic force microscope tip and a C atom of graphene on SiC(0001) is exposed to an external electric field. For one field orientation the Au-C bond is strong enough to sustain the mechanical load of partially detached graphene, whilst for the opposite orientation the bond breaks easily. Calculations based on density functional theory and nonequilibrium Green's function methods support the experimental observations by unveiling bond forces that reflect the polar character of the bond. Field-induced charge transfer between the atomic orbitals modifies the polarity of the different electronegative reaction partners and the Au-C bond strength.

O 93.2 Thu 10:30 P

Simulating the scattering of a hydrogen atom from graphene using a high-dimensional neural network potential. — •Sebastian Wille[1,2,3], Hongyan Jiang[2], Oliver Bünermann[2], Alec M. Wodtke[1,2], Jörg Behler[3], and Alexander Kandratsenka[2] — [1]Institute for Physical Chemistry, Georg-August University Göttingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany — [3]Theoretical Chemistry, Georg-August University Göttingen, Germany

Understanding the formation of covalent bonds due to atomic-scale motions and energy dissipation pathways involved is an ongoing challenge in the field of chemistry. Measurements performed in our group show a bimodal pattern of the translational energy loss distribution of hydrogen atoms scattered from graphene. The second generation reactive empirical bond order potential was fitted to ab initio electronic structure data obtained from embedded mean-field theory to generate a potential energy surface (PES). First-principles dynamics simulations using the provided PES were able to reproduce the bimodal feature of the energy loss spectrum and were in qualitative agreement with experimental results. But these investigations could not fully provide a detailed description of the scattering and sticking mechanisms. Therefore, we developed a full-dimensional neural network PES by fitting to the density functional data in order to further reduce the remaining errors by the fitting procedure of the PES underlying molecular dynamics simulations performed, which better fits the experiment.

O 93.3 Thu 10:30 P

Intercalation of silver between graphene and silicon carbide studied by PEEM and AFM — •Philipp Weinert[1,2], Richard Hönig[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — [2]DELTA, TU Dortmund, Maria-Goeppert-Mayer Straße 2, 44227 Dortmund, Germany

Due to its outstanding electronic, magnetic, and mechanical properties graphene is of particular interest multiple fields.

In this study the intercalation of silver between one layer of graphene, the so-called buffer layer, and a silicon carbide substrate is investigated. Other studies have shown that covalent bounds between the silicon carbide and the buffer layer are released by intercalation, which leads to quasi free standing graphene.

To achieve the intercalation, samples have been coated with thin silver-films of different and defined thicknesses. Subsequently, the samples have been annealed to initiate the intercalation. In different steps of the annealing process, photoemission electron microscopy (PEEM) has been carried out to investigate the work function of the surface. This investigation has proven that silver intercalated underneath the buffer layer during the annealing. Moreover, in the case of thick silver layers a contrast inversion was visible. Furthermore, atomic force microscopy (AFM) has been carried out to investigate the topography of the samples after the intercalation. This study has shown that a small part of the silver does not intercalate, but forms islands on the surface.

O 93.4 Thu 10:30 P

Modeling the self-assembly of graphene flakes on liquid Cu — •Juan Santiago Cingolani, Mie Andersen, and Karsten Reuter — Chair of Theoretical Chemistry, Technical University of Munich, Germany

The use of liquid Cu as a catalyst for the production of graphene during chemical vapor deposition has been shown to lead to high-quality single layer millimeter-scale graphene flakes. In-situ optical microscopy revealed that the flakes are mobile on the liquid surface and interact with each other leading to the formation of self-assembled structures. We carry out a series of molecular dynamics simulations of graphene flakes on liquid Cu employing the third-generation charge optimized many body potential (COMB3) to shed some light on the origin of such inter-flake interactions.

From our simulations we extract information regarding the interaction of the flakes with the liquid substrate; namely the adsorption height, interaction energy, and charge transfer into the adsorbate. We extrapolate these properties to the limit of large flakes and use them as input for a mesoscopic model which accounts for electrostatic repulsion and capillary attraction assuming charged spherical particles. The resulting interaction potential predicts interflake distances within an assembly that lie within an order of magnitude of the experimental observations. While quantitative agreement is out of the scope for such a simple model, we show that the experimental observations are compatible, under the proposed mesoscopic model, with the microscopic properties derived from atomistic simulations.

O 93.5 Thu 10:30 P

Reduced step bunching during growth of epitaxial graphene on silicon carbide (0001) — •Robert Appel, Philipp Weinert, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Strasse 4a, 44227 Dortmund, Germany

Epitaxial graphene (EG) has attracted significant interest in the recent years due to the simple preparation method by heating silicon carbide (0001). The major drawback of this approach is step bunching (SB) that leads to large terraces and tall step heights. These disconnect the EG layers from step to step resulting in anisotropic electronic and magnetic properties. To prevent this, samples with shallow steps are desired. The $(6\sqrt{3} \times 6\sqrt{3})$R30°-reconstruction (so-called buffer layer (BL)) of the SiC(0001) constrains the SB and forms while heating. Therefore, a fast formation of the BL while heating without mono layer or bilayer patches is of utmost importance.

We use the confinement controlled sublimation (CCS) method in argon atmosphere because it is known for reproducibility and tunability. Thus, it is a promising method to find the ideal parameters for fast BL formation. Kruskopf et al. demonstrated the preparation of EG with shallow steps and less SB by using a high heating rate, a short heating time and a high preparation temperature.

In this study, we explore the applicability of the CCS method in order to obtain similar results with shallow steps and less SB. For this purpose, we systematically modify the preparation parameters and characterize the obtained samples with atomic force microscopy.

O 93.6 Thu 10:30 P

Influence of Chemical Interactions on Low Energy Ion bombardment of 2D Materials: Insights from ab-initio Molecular Dynamics — •Silvan Kretschmer[1], Sadegh Ghaderzadeh[1], and Arkady V. Krasheninnikov[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Department of Applied Physics, Aalto University, Finland

Low energy ion implantation (LEII) provides a valuable tool to tune the mechanical, electronic and catalytic properties of 2D materials by the targeted implantation of impurities. In contrast to ion irradiation at higher energies the commonly applied binary collision formula fails to describe the outcome of the irradiation process for ions close to the displacement energy, that is the minimum ion energy needed to displace the target atom. The dominating influence of the chemical interaction of projectile and target atoms and its effect on the displacement energy are addressed in this work. For that, we carried out ab-initio molecular dynamics (MD) simulations for a broad range of projectiles (elements Hydrogen to Argon) impacting on graphene and h-BN, and determined the energies needed to displace C, N and

B atoms, respectively. We further present and validate a scheme to incorporate the effect of spin-polarization on the displacement process - as spin-polarized ab-initio MD runs tend to fail at bond-breaking.

O 93.7 Thu 10:30 P

hBN/Pt(111) and hBN/Ir(111): distinctive templates for Cs adsorption — •Jiaqi Cai, Robin Ohmann, and Carsten Busse — Department Physik, Universität Siegen, Walter-Flex-Str. 3, 57072 Siegen

High-quality two-dimensional materials (2DM) can be grown by epitaxial methods on the high-symmetry surfaces of transition metal crystals. This epitaxy leads to the interaction between 2DMs with the underlying substrate, which periodically modulates their geometric and electronic structure. This spatial periodicity constitutes a moiré pattern.

The periodic electronic modulation of the moiré pattern provides a template for adsorbates. To study this templating effect, we deposit Cs onto hBN/Pt(111) and hBN/Ir(111). Our scanning tunneling microscopy measurements reveal, hBN/Pt(111) and hBN/Ir(111) are very different templates: the preferred adsorption sites on hBN/Pt(111) are the strongly bonded regions (valleys) of the moiré unit cell, and on hBN/Ir(111) the weakly bonded regions (hills). Furthermore, one valley region on hBN/Pt(111) can accommodate multiple alkali metal atoms, while only one single Cs atom can adsorb on the hill of the hBN/Ir(111) moiré unit cell. An additional feature of Cs adsorption on hBN/Ir(111) is that there are two hill regions in one moiré unit cell. With the proper preparation procedure, the adsorbed Cs atoms form an unusual honeycomb lattice.

O 93.8 Thu 10:30 P

Preparation of antimony monolayers on Ag(111) — •Stefanie Hilgers[1], Julian A. Hochhaus[1,2], Anneke Reinold[1], Malte G. H. Schulte[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Str. 4a, 44227 Dortmund, Germany — [2]DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227, Dortmund, Germany

In the here presented research, we prepare and investigate antimony monolayers on Ag(111). Similar to graphene, the elements of the 5th main group such as phosphorus, arsenic, and antimony are predicted to have extraordinary electronic properties.

Due to the small lattice mismatch between silver and free-standing antimonene, Ag(111) is a suitable substrate for the preparation of antimony monolayers. The substrate was cleaned by argon sputtering and heating in UHV, while the antimony monolayers were prepared by molecular beam epitaxy (MBE). Auger electron spectroscopy (AES) was used to investigate the chemical surface composition, while structural investigations were carried out using low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) at room temperature.

O 93.9 Thu 10:30 P

Preparation and characterization of lead monolayers on Pd(111) — •Anneke Reinold[1], Julian Hochhaus[1,2], Ismail Baltaci[1], Stefanie Hilgers[1], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Str. 4a, 44227 Dortmund, Germany — [2]DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund, Germany

The research presented here focuses on the preparation of lead monolayers on Pd(111). With the experimental realization of two-dimensional lead by Yuhara et al. in 2019, the field of 2D materials was recently expanded. According to theoretical predictions, the so-called plumbene has the largest band gap and the highest spin-orbit coupling from all group 14 elements due to its high mass. Additionally, plumbene was predicted to show the quantum spin Hall effect (QSHE) even at room temperature. Therefore, plumbene is an ideal candidate for topological insulators and future electronic applications.

We want to achieve a more detailed knowledge of the behavior of different layer thicknesses of lead on palladium. We prepared Pd(111) by repeated cycles of argon sputtering and heating. The monolayers were deposited by thermal vapor deposition. Low-Energy Electron Diffraction (LEED) and Scanning Tunneling Microscopy (STM) were used to characterize the Pb/Pd(111) system.

O 93.10 Thu 10:30 P

Ultrathin oxide/graphene heterostructures — •Andrea Picone — Department of Physics, Politecnico di Milano, Milano, Italy

Graphene interfaced with oxide ultrathin films is a particularly appealing system for the development of new devices, since the dielectric layer can be used to modulate the physical properties of the carbon monolayer. Furthermore, graphene can be used as a template to synthesize novel two-dimensional oxide materials.[1] Despite such an extreme technological and scientific interest, only few successful examples of sharp graphene/oxide interfaces have been reported so far, since the growth of atomically flat ultrathin oxide films on the honeycomb monolayer is hampered by the extremely low surface free energy of graphene, which promotes the nucleation of three-dimensional clusters. Here, by using standard surface science techniques, I will analyze the structural, chemical and electronic properties of transition metals oxide (CrxOy and FexOy) and rare earths oxide (ErxOy)ultrathin films grown on the graphene/Ni(111) substrate.[2,3] The experimental results reveal a rich variety of graphene heterostructures, depending on the element used and the synthesis procedure.

[1] Netzer, F. P.; Surnev, S. Oxide Materials at the Two-Dimensional Limit; Springer, (2016)

[2] Lodesani, A. ; Picone, A.; Brambilla, A.; Giannotti, D.; Jagadeesh, M.S.; Calloni, A.; Bussetti, G.; Berti, G.; Zani, M.; Finazzi, M.; Duò, L.; Ciccacci, F. ACS Nano 13, 4361-4367 (2019)

[3] Lodesani, A.; Picone, A.; Brambilla, A.; Finazzi, M.; Duò, L.; Ciccacci, F. J. Chem. Phys. 152, 054706 (2020)

O 93.11 Thu 10:30 P

Kinetic nanoscale friction and intermittent hybridization in graphene stacks on SiC — •Bartosz Szczefanowicz[1], Leonhard Mayrhofer[2], Andreas Klemenz[2], Michael Moseler[2], and Roland Bennewitz[1] — [1]INM - Leibniz Institute for New Materials, Saarbrücken, Germany — [2]IWM Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany

Graphene is an excellent lubricant on micro- and nanoscale due to its weak normal-to-plane interactions. Friction Force Microscopy (FFM) demonstrated ultralow friction for graphene on many different substrates. However, the friction force for epitaxial graphene on SiC(0001) increases dramatically above a normal load threshold [1]. We suggest that the observation can be explained by a pressure-induced temporal and local orbital rehybridization from sp^2 to sp^3 and a corresponding change of interlayer van der Waals interaction into metastable covalent bonds [2].

We report friction force measurements for graphene/SiC(0001) in ultrahigh vacuum as function of normal load and sliding rate and compare the results to atomistic simulations based on density functional theory (DFT). An excellent agreement of the load-dependence reveals friction mechanisms involving pressure-induced intermittent bonds.

[1] T. Filleter, R. Bennewitz, Physical Review B, 81 (2010), 155412

[2] Y. Gao, et al, Nature Nanotechnology, 13 (2018), 133-+.

O 93.12 Thu 10:30 P

Hetero-Stacking of 2D Materials by Sequential Chemical Vapour Deposition — •Nicolas Néel, Alexander Mehler, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

A multi-step method that enables the growth of graphene on hexagonal boron nitride (h-BN) on Pt(111) is presented. Using borazane (BNH6) as a molecular precursor, h-BN is grown on the surface in the first step. In a next step, a sufficiently thick Pt film is adsorbed and buries the h-BN mesh. It acts as a catalyst for the subsequent growth of graphene via the chemical vapour deposition of ethylene (C2H4). The last step involves the thermally induced entire intercalation of the Pt film beneath h-BN giving rise to large surface regions of a graphene/h-BN stacking. A unique moiré superstructure results from the h-BN-Pt interface. Upon reducing the tip-sample separation an additional $\sqrt{3} \times \sqrt{3}\,\mathrm{R}\,30^\circ$ superlattice gradually appears.

O 93.13 Thu 10:30 P

In-plane heterostructures of transition metal dichalcogenide monolayers — •Kai Mehlich[1,2], Daniela Dombrowski[1,2], Thais Chagas[1], Daniel Kurz[1], Thomas Michely[3], and Carsten Busse[1] — [1]Department Physik, Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen — [2]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [3]II. Physikalisches Institut , Universität zu Köln, Zülpicher Str. 77, 50937 Köln

Modern electronics and optoelectronics utilise complex materials to maximize efficiency and reduce size, while requiring specific electronic properties. 2D-materials can fulfill these desires excellently. With epitaxial growth of monolayer transition metal dichalcogenides like TaS_2,

WS_2 and MoS_2 already an established line of research, we increased the range of possibilities by successfully growing in-plane heterostructures of these materials. The heterostructures are realised by sequential epitaxial growth of monolayers on Au(111), thereby forming the thinnest possible heterostructures. The material combination was chosen because of the difference in lattice parameters and electronic structure (as monolayer MoS_2 and WS_2 are semiconductors and monolayer TaS_2 is metallic). The difference in lattice parameters induces stress, which has to be compensated. We categorised the relieve mechanisms into three groups, being: Defects, compression or stretching of the materials, and deformation in the z-plane. The mechanisms are observed by STM-imaging and analysed quantitatively on their appearance depending on the hetero-boundary, mostly showing an uninterrupted boundary.

O 93.14 Thu 10:30 P

Catalytically assisted growth of molybdenum disulfide monolayers on silicon dioxide substrates — Ana Burgos[1], Valeria Del Campo[1], and •Patricio Häberle[1,2] — [1]Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso 2390123, Chile — [2]Institute of Applied Physics, Vienna University of Technology, 1040 Vienna, Austria

MoS2 monolayers grown by chemical vapor deposition (CVD), starting from MoO3 and S precursors, occurs mostly in form of patches over the substrates, leaving some sections nearly clean. There is a large heterogeneity of the resulting products, regarding size and shape of the structures, obtained. We have explored, the formation of MoS2 layers grown by CVD on silicon dioxide substrates, while exposed to HOPG (Highly Oriented Pyrolytic Graphite). HOPG provides a catalytic surface that promotes the chemical reactions involved in the formation of MoS2. We have proposed a detailed model of the chemical reactions involved in this monolayer growth. It proceeds via the formation of MoO2 on the HOPG surface, followed by the gas phase synthesis of MoS2, which is subsequently collected over the substrate. Our analysis, using optical microscopy and Raman spectroscopy of the resulting products, indicate that the ratio between MoO2 and S is a crucial variable in the formation of monolayers. A set of optimal experimental conditions were established in order to promote homogeneous growth of MoS2 monolayers.