O 36: Poster: 2D Materials II

Time: Tuesday 18:00–20:00 Location: P2/EG

O 36.1 Tue 18:00 P2/EG

Simulation of proximity effects in epitaxial graphene systems — •Andres David Peña Unigarro[1], Florian Steffen Günther[2,3], and Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz, Chemnitz, Germany — [2]IFSC, University of São Paulo, Brazil — [3]UNESP, Brazil

Two-dimensional materials such as graphene are fascinating because they combine mechanical flexibility with unique electronic properties. The next level of complexity, however, comprises the assembly of various 2D materials to generate structures with enhanced characteristics. Using proximity effects, changes in the electronic, optical and transport properties of epitaxial graphene have been produced while preserving the regular honeycomb structure that can be grown on silicon carbide, SiC. Such modifications can, for instance, be achieved by proximity effects in hetero stacks with intercalate and absorbate layers with other 2D materials or by the presence of a functional integration environment. In the past years, many elements were intercalated below the graphene sheet, forming partly well-defined hetero bilayer systems with different functionalities. As suggested by density functional theory (DFT) studies, elements of the IV group can be used for this purpose. In this case, intercalation of heavy atoms like Pb are expected to introduce additional effects such as spin-orbit coupling to the electron gas of graphene. In this contribution, we present preliminary results obtained with DFT focusing on the study of modifications of the electronic structure of epitaxial graphene due to proximity effects generated by the intercalation of Pb on buffer layers on SiC.

O 36.2 Tue 18:00 P2/EG

Structural Characterization of a Novel Two-Dimensional Material: Cobalt Sulfide Sheets on Au(111) — •Marcel Rost[1], Mahesh Prabhu[2], Dajo Boden[2], Jörg Meyer[2], and Irene Groot[2] — [1]Huygens-Kamerlingh Onnes Laboratory, Leiden Institute of Physics, Leiden University, 2300 RA Leiden, The Netherlands — [2]Leiden Institute of Chemistry, Leiden University, P.O. Box 9502, 2300 RA Leiden, The Netherlands

Transition metal dichalcogenides (TMDCs) are a type of two-dimensional (2D) material that has been widely investigated by both experimentalists and theoreticians because of their unique properties. In the case of cobalt sulfide, density functional theory (DFT) calculations on free-standing S-Co-S sheets suggest there are no stable 2D cobalt sulfide polymorphs, whereas experimental observations clearly show TMDC-like structures on Au(111). In this study, we resolve this disagreement by using a combination of experimental techniques and DFT calculations, considering the substrate explicitly. We find a 2D CoS(0001)-like sheet on Au(111) that delivers excellent agreement between theory and experiment. Uniquely this sheet exhibits a metallic character, contrary to most TMDCs, and exists due to the stabilizing interactions with the Au(111) substrate.

O 36.3 Tue 18:00 P2/EG

Carbon Nanomembranes Fabricated from Amorphous Molecular Layers — •Zhen Yao[1], Nikolaus Meyerbröker[2], Yubo Qi[1], Michael Westphal[1], Yang Yang[1], and Armin Gölzhäuser[1] — [1]Bielefeld University, Bielefeld, Germany — [2]CNM Technologies, Bielefeld, Germany

Ultrathin carbon nanomembranes (CNMs), fabricated from crosslinking self-assemblies of molecular precursors, are 2D membranes that possess well-defined physical and chemical properties. With a simple transfer procedure, CNMs can be placed on various supports, enabling versatile applications. Combining high water flux and precise ion selectivity, CNMs are ideal materials for molecular separation and water desalination. However, their practical realization is hindered by the availability of epitaxial metal substrates. Here, we report a new type of CNM fabricated from poly(4-vinylbiphenyl) (PVBP) spin-coated on SiO2/Si substrate. The electron-induced crosslinking results in the formation of a continuous membrane with a thickness of 15 nm. The nanoporous nature of the PBVP-CNM is revealed by water and ion permeation measurements. The membrane possesses a high density of pores, which allows water flux as high as 530 L m-2 h-1 bar-1. It also exhibits the rejection of ions and molecules with sizes >1 nm. A further introduction of a reinforcement porous block copolymer layer simplifies the transfer procedure, resulting in a centimetre-scale CNM-composite that works efficiently for dye rejection. These results suggest a feasible route for large-scale nanoporous membrane fabrication.

O 36.4 Tue 18:00 P2/EG

A New Group of Two-Dimensional Non-van der Waals Materials with Ultra Low Exfoliation Energies — •Tom Barnowsky[1,2], Arkady V. Krasheninnikov[1,3], and Rico Friedrich[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Theoretical Chemistry, Technische Universität Dresden, 01062 Dresden, Germany — [3]Aalto University, Aalto 00076, Finland

The exfoliation energy, *i.e.* the energy required to separate a single two-dimensional (2D) sheet from a bulk material, is a key factor in whether such 2D systems can be made. Recently, non-van der Waals 2D compounds – materials derived from non-layered bulk counterparts – were outlined as a rich new class of nanoscale materials [1].
In our work, using data-filtering and ab-initio calculations, we propose a group of eight novel non-van der Waals 2D systems [2]. The compounds exhibit ultra-low exfoliation energies close to those of traditional van der Waals bound 2D materials. Especially for the considered sulfides, strong surface relaxations play a key role in the energy gain enabling exfoliation, while the effects of long-range dispersive interactions are minor. The candidates with the smallest exfoliation energies, 2D $SbTlO_3$ and $MnNaCl_3$, exhibit appealing electronic, potential topological, and magnetic features as evident from the calculated band structures.

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

O 36.5 Tue 18:00 P2/EG

Magnetic properties of transition metal dihalides measured by x-ray magnetic circular dichroism (XMCD) — •Sebastien Elie Hadjadj[1], Samuel Kerschbaumer[2], Andrea Aguirre Banos[3], Danilo Longo[3], Fadi Choueikani[4], Celia Rogero[2], Jose Ignacio Pascual[3], Wolfgang Kuch[1], and Maxim Ilyn[2] — [1]Institut für Experimentalphysik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Centro de Fisica de Materiales (CSIC/UPV-EHU), 20018 Donostia-San Sebastian, Spain — [3]CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastian, Spain — [4]Synchrotron SOLEIL, 91190 Saint-Aubin, France

During the last couple of years, there has been a rising interest in novel two-dimensional magnetic materials. Most recently, several groups have shown that magnetic order in two-dimensional materials can be stable [1]. Here we report the single phase epitaxial growth of ML to multilayer CoBr2 and CoCl2 Au(111) as well as on NbSe2. The samples where characterized via LEED, XPS, XAS, XMCD and LT-STM. Both Co-compounds show a strong in-plane anisotropy and ferromagnetic order up to temperatures of around 20 K.

[1] Djuro Bikaljevic et al., ACS Nano, 15, 14985 (2021)

O 36.6 Tue 18:00 P2/EG

Silicene's pervasive surface alloy on Ag(111) — Johannes T Küchle[1,2], Aleksandr Baklanov[1], Ari P Seitsonen[3,4], Paul TP Ryan[2,5], Peter Feulner[1], Prashanth Pendem[1], Tien-Lin Lee[2], Matthias Muntwiler[6], Martin Schwarz[1], Felix Haag[1], Johannes V Barth[1], Willi Auwärter[1], •David A Duncan[1,2], and Francesco Allegretti[1] — [1]Physics Department E20, Technische Universität München, Deutschland — [2]Diamond Light Source, Oxfordshire, UK — [3]Département de Chimie, École Normale Supérieure, Paris, France — [4]Université Paris Sciences et Lettres, Sorbonne Université, Paris, France — [5]Imperial College London, UK — [6]Paul Scherrer Institut, Villigen, Switzerland

Silicene is the two-dimensional (2D) allotrope of silicon. So far, the most direct synthesis strategy has been to grow it epitaxially on metal surfaces; however, the effect of the strong silicon-metal interaction on the structure and electronic properties of the metal-supported silicene is generally poorly understood. Here, we consider the (4×4)-silicene monolayer (ML) grown on Ag(111), and show that our experimental results refute the common interpretation of this system as a simple buckled, honeycomb ML with a sharp interface to the Ag substrate. Instead, we demonstrate the pervasive presence of a second silicon

species, concluded to be a Si/Ag alloy stacked between the 2D silicene and the silver substrate. These findings question the current structural understanding of the silicene/Ag(111) interface and may raise expectations of analogous alloy systems in the stabilization of other 2D materials grown epitaxially on metal surfaces.

O 36.7 Tue 18:00 P2/EG

Pb-induced proximity effects in epitaxial graphene — Andres David Pena Unigarro, Chitran Ghosal, •Christoph Tegenkamp, and Sibylle Gemming — Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, 09126 Chemnitz

A current topic in material science deals with the controlled assembly of various 2D materials to generate structures with new quantum characteristics. Such modifications can be achieved by proximity effects, e.g., by intercalation and adsorption. One promising route is to use epitaxial buffer layer structures on SiC(0001) surfaces, which transforms into a quasi free monolayer graphene with new 2D interface structures upon intercalation. As suggested by density functional theory (DFT) studies, elements of the IV group such as Pb can be used for this purpose. In this case, intercalation of heavy atoms like Pb are expected to introduce additional effects such as spin-orbit coupling to the electron gas of graphene. In this contribution, we investigated the intercalation of Pb on buffer layers on SiC(0001). Suspended and charge neutral graphene emerged, and the intercalated Pb formed plumbene honeycomb lattices, which are rotated by 7.5° with respect to graphene. Along with this twist, a proximity-induced modulation of the hopping parameter in graphene opens a band gap of around 30 meV at the Fermi energy, giving rise to a metal-insulator transition. We present first results obtained with DFT focusing on the modifications of graphene's electronic structure in the presence of twisted Pb layers.

O 36.8 Tue 18:00 P2/EG

Local spectroscopy of acoustic phonons in low-dimensional materials — •Yi Zhang[1], Shaoxiang Sheng[1,2], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Coherent acoustic phonons (CAPs) enable ultrafast control of solids and have been exploited for applications in various acoustic devices. THz-induced ultrafast Coulomb forces in a scanning tunnelling microscope (STM) junction can locally generate CAP wave packets that propagate with low losses and form longitudinal acoustic standing waves in a thin Au film on mica [1,2]. Here we develop a discrete lattice model to simulate acoustic phonon propagation in well-defined nanostructures. We predict that transverse acoustic phonons can be detected in 1D chains or in 2D thin films by THz-STM. This enables investigation of mechanical properties and electron-phonon interaction in nano-materials at the atomic scale. [1] S. Sheng, et al. Physical Review Letters 129, 043001 (2022). [2] M. Abdo, et al. ACS Photonics 8, 702-708 (2021).

O 36.9 Tue 18:00 P2/EG

Structure and electronic properties of antimonene on Ag(111) — •Friedrich Wanierke, Felix Otto, Maximilian Schaal, Marco Grünwald, Lorenz Brill, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University jena, Helmholtzweg 5, 07743 Jena

The synthesis of new two-dimensional (2D) materials is of great interest for the development of new designs of electronic devices. In this study, we payed special emphasis on the growth of the elemental 2D semiconductor antimonene on Ag(111) by molecular beam epitaxy. To characterize and evaluate the deposited films, we used various methods of surface science. On the one hand, we performed in situ reflection high energy electron diffraction (RHEED), low energy electron diffraction (LEED) and low-temperature scanning tunneling microscopy (STM) for structural investigations. On the other hand, photoelectron spectroscopy as well as STM were used to reveal the electronic properties of the ultra-thin films. The alloy Ag_2Sb, as well as β- and α-antimonene, with respect to the amount of deposited antimon, are discussed.

O 36.10 Tue 18:00 P2/EG

Impact of screening and relaxation on weakly coupled 2D heterostructures: implications for molecular spin-coupling — Eva Rauls[1], T.T. Nhung Nguyen[2], Christoph Tegenkamp[2], and •Uwe Gerstmann[3] — [1]University of Stavanger, Norway — [2]Technische Universität Chemnitz, Germany — [3]Universität Paderborn, Germany

Phthalocyanines (Pc) at surfaces are prototype molecules which can host magnetic ions in a well-defined surface environment. The precise external control of individual spins, however, require a detailed knowledge of the influence of the substrate. In this combined experimental and theoretical study, we have investigated the influence of different graphene-related substrates onto the structural, electronic and magnetic properties of adsorbed Pb and Mn-phthalocyanines. Formation of almost identical densely packed PbPc molecular layers with strongly tilted molecules were found on *n*-type and *p*-type doped 2D templates. On graphite (HOPG), the dispersing molecular states of the less deformed molecular adsorbate stress the importance of substrate mediated interaction and proximity coupling [1]. After substituting Pb by magnetic Mn, the interaction with the substrate is clearly increased. On epitaxial monolayer graphene (MLG) the MnPc experience even the underlying SiC substrate, resulting in a 4×2 reconstructed molecular layer with very specific substrate mediated magnetic coupling.

[1] T.T. Nhung Nguyen, T. Sollfrank, C. Tegenkamp, E. Rauls, U. Gerstmann, Phys. Rev. B 103, L201408 (2021).

O 36.11 Tue 18:00 P2/EG

Honeycomb structure of alkali metal atoms — Jiaqi Cai[1,2,3], •Robin Ohmann[1], Nicolae Atodiresei[4], Hai Chau Nguyen[1], David Duncan[5], Caio Silva[2], Christoph Schlueter[5], Kai Mehlich[1], Thais Chagas[1], Vasile Caciuc[4], Wouter Jolie[3], Stefan Blügel[4], Tien-Lin Lee[5], Thomas Michely[3], and Carsten Busse[1,2,3] — [1]Department Physik, Universität Siegen, Siegen, Germany — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany — [3]II. Physikalisches Institut, Universität zu Köln, Köln, Germany — [4]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, Jülich, Germany — [5]Diamond Light Source, Didcot, Oxfordshire, United Kingdom

The formation of honeycomb structures, similar to graphene, is of great scientific and technological interest. Here, we show that the adsorption of Cs on monolayer hexagonal boron nitride (hBN) on Ir(111) substrate kept at elevated temperatures forms a honeycomb lattice. The structure is investigated by scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and X-ray standing waves (XSW) revealing that the Cs atoms are in registry with the moiré pattern of the substrate with a lattice constant of about 30 Å, are partially positively charged and have an adsorption height of 2.9 Å above the hBN layer. The formation is explained via the templating effect of the substrate. Our density functional theory (DFT) results confirm stable binding on the two hill regions of the moiré unit cell and predict a graphene like band structure with a band width of about 1 meV.

O 36.12 Tue 18:00 P2/EG

Unstrained Sb Bilayers on InSb(111)A — Bing Liu[1,2], •Stefan Enzner[1,3], Tim Wagner[1,2], Philipp Eck[1,3], Martin Kamp[2], Giorgio Sangiovanni[1,3], and Ralph Claessen[1,2] — [1]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany

Antimonene, a hexagonal arrangement of staggered Sb, is a promising topological material, which has been widely investigated on various substrates. Recently, it has been grown strain-free on InSb(111)A by forming a moiré structure, despite exhibiting covalent interface bonds.

The moiré supercell is theoretically approximated with varying interface stackings of primitive cells by means of ab initio DFT calculations. This approach reproduces the main structural and electronic observations. The agreement allowed us, to investigate the competition of intra-layer and interface interactions and explain the reconstruction-free growth.