

O 74: 2D Materials IV: Heterostructures (joint session O/CPP)

Time: Thursday 10:30–12:45

Location: GER 37

O 74.1 Thu 10:30 GER 37

In-situ growth characterization of 2D heterostructures: MoSe₂ on intercalated graphene/Ru(0001) — ●LARS BUSS¹, NICOLAS BRAUD², MORITZ EWERT¹, MATTEO JUGOVAC³, TEVFIK ONUR MENTES³, ANDREA LOCATELLI³, JENS FALTA², and JAN INGO FLEGE¹ — ¹Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — ²Institute for Solid State Physics, University of Bremen, Bremen, Germany — ³Eletra-Sincrotrone Trieste S.C.p.A, Bazovizza, Trieste, Italy

Despite the great fundamental interest in 2D heterostructures, most of the investigated 2D heterostructures were realized by mechanical exfoliation or chemical vapor deposition in the millibar range, preventing true in-situ characterization of the growth process. Here, we have investigated the growth of MoSe₂ on single-layer graphene on Ru(0001) via real-time in-situ low-energy electron microscopy and micro-diffraction. After preparation of the graphene by standard procedures from an ethylene precursor, MoSe₂ has been prepared via co-deposition of Mo and Se. Prior Se intercalation of the graphene appears to enhance the subsequent growth of MoSe₂ on the graphene. At elevated temperatures, rotational ordering of the MoSe₂ is facilitated by the strongly enhanced mobility of single-domain MoSe₂ islands that align with the high symmetry orientations of the underlying graphene, indicating a non-negligible interaction between the two van-der-Waals materials. Micro-spot angle-resolved photoemission proves the monolayer nature of the as-grown MoSe₂ as well as the free-standing character of the Se-intercalated graphene underneath.

O 74.2 Thu 10:45 GER 37

Designer quantum states in metal-organic frameworks — ●ORLANDO J SILVEIRA¹, LINGHAO YAN¹, SHAWULIENU KEZILEBIEKE², BENJAMIN ALLDRITT¹, VILIAM VANO¹, ONDŘEJ KREJČÍ¹, JOSE LADO¹, ADAM S FOSTER^{1,3}, and PETER LILJEROTH¹ — ¹Department of Applied Physics, Aalto University, Espoo, Finland — ²University of Jyväskylä, FI-40014 University of Jyväskylä, Finland — ³Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Vertical heterostructures have emerged as a promising path to the design of quantum materials with exotic properties. Here, we show that this concept can be also extended to a family of 2D kagome metal-organic frameworks (MOFs) of the family M₂DCA₃, with M= Cu and Ni. The two MOFs have been fabricated either on a graphene/Ir(111) surface or the superconducting substrate NbSe₂, and the structural and electronic properties of different phases of both 2D MOFs + substrates were studied through density functional theory (DFT) calculations. Results show that the Cu₂DCA₃ MOF is effectively decoupled from the Ir(111) metallic substrate by the graphene layer, which is important to reveal the topological properties of this family of MOF. Moreover, this study extends the synthesis and electronic tunability of 2D MOFs beyond the metal surfaces to superconducting substrates, which are needed for the development of emerging quantum materials. We show that the Ni₃DCA₂ MOF has a spin density around the Ni atom when synthesized on the NbSe₂ substrate due to charge transfer, and this makes a perfect platform to realize topological superconductivity.

O 74.3 Thu 11:00 GER 37

Phonon gap supported tunneling and Faraday screening through graphene — ●TOBIAS WICHMANN^{1,2,3}, KEDA JIN^{1,2,4}, JOSE MARTINEZ CASTRO^{1,4}, HONEY BOBAN⁵, LUKASZ PLUCINSKI⁵, MARKUS TERNES^{1,2,4}, F. STEFAN TAUTZ^{1,2,3}, and FELIX LÜPKE^{1,2} — ¹Peter-Grünberg-Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — ²Jülich Aachen Research Alliance (JARA) - 52425 Jülich, Fundamentals of Future Information Technology, Germany — ³Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany — ⁴Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany — ⁵Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany

Encapsulation of van der Waals materials has proven a vital technique to protect them from degradation and contamination. Usually, metallic encapsulation layers mask the properties of the underlying material when studied in scanning tunneling microscopy. Utilizing the inelastic tunneling phonon gap of graphene, however, enables the unfettered investigation of low energy phenomena (e.g. Kondo effect, Majoranas,

etc.) by scanning tunneling spectroscopy, while maintaining the advantages of encapsulated samples. Furthermore, we find that the conductive nature of the graphene encapsulation layer screens the sample from tip-induced electric fields, exemplified by our low-temperature STM examination of encapsulated Fe₃GeTe₂.

O 74.4 Thu 11:15 GER 37

Fermi level tuning of a MnBi₂Te₄ monolayer — ●MARCO DITTMAR¹, PHILIPP KAGERER¹, CELSO I. FORNARI¹, SIMON MÜLLER¹, SERGIO L. MORELHÃO², HENDRIK BENTMANN¹, and FRIEDRICH REINERT¹ — ¹Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany — ²Instituto de Física, Universidade de São Paulo, Brazil

By breaking time reversal symmetry, introducing magnetic order to topological insulators leads to the opening of a 2D surface state gap at the Dirac point. As a second crucial parameter, tuning the position of the Fermi level inside this gap, enables the observation of exciting new phenomena, such as the quantum anomalous Hall effect (QAHE). Here, we focus on the intrinsic ferromagnetic monolayer of MnBi₂Te₄, acting as a magnetic extension of the topological insulator Bi₂Te₃ [1]. We tune the Fermi level position in this compound by preparing a single layer of MnBi₂Te₄ on top of the topologically non-trivial p-n-junction of Sb₂Te₃ and Bi₂Te₃ grown by molecular beam epitaxy (MBE) [2]. We will present a study containing structural characterization of the heterostructures by X-ray diffraction and atomic force microscopy, while the electronic structure is assessed by X-ray and angle resolved photoemission spectroscopy.

[1] M. M. Otrokov *et al.*, 2D Mater 4, 025082 (2017)[2] P. Kagerer *et al.*, arXiv 2207.14421 (2022)

O 74.5 Thu 11:30 GER 37

1D Topological Superconductivity in a van der Waals heterostructure probed by Abrikosov vortices — ●JOSE MARTINEZ-CASTRO^{1,2}, TOBIAS WICHMANN^{1,3}, TOMÁŠ SAMUELY⁴, KEDA JIN^{1,2}, OLEKSANDER ONUFRIENKO⁴, F. STEFAN TAUTZ^{1,3,5}, MARKUS TERNES^{1,2,3}, and FELIX LÜPKE¹ — ¹Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — ²Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany. — ³Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, 52425 Jülich, Germany — ⁴Centre of Low Temperature Physics, Faculty of Science, P. J. Safarik University & Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia — ⁵Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany

The 2D topological insulator monolayer (ML) WTe₂ is characterized by an insulating interior surrounded by helical 1D edge states. When this material is brought into proximity to the s-wave superconductor NbSe₂, the spectroscopic features of the helical edge state remain intact while showing a proximity-induced superconducting gap [1]. However, so far there has been no direct evidence that the observed edge superconductivity is of different nature than that observed away from the edge. Here, by inducing Abrikosov vortices at the boundary between ML WTe₂ and NbSe₂, we show that the induced superconductivity in the helical edge is robust against magnetic fields, a strong indication of 1D topological superconductivity.

[1] Lüpke *et al.*, Nat. Phys. 16, 526 (2020)

O 74.6 Thu 11:45 GER 37

Density functional theory studies of Anthracene on MoS₂ — ●GÉRALD KÄMMERER and PETER KRATZER — Faculty of Physics, University of Duisburg-Essen

Thin layers of MoS₂ are attractive as transparent contacts on organic semiconductors, e.g., oligoacene. As a model for molecules with a delocalized system of π -bonds, we investigate the physisorption of a monolayer of anthracene (C₁₄H₁₀) on a MoS₂ single layer using density functional theory. The calculations were carried out with the FHI-Aims code with different functionals. Van der Waals interactions are described by a pairwise potential of the Tkatchenko-Scheffler type or by a many-body dispersion technique. We determine structural properties and can identify the relative position of the molecular HOMO and LUMO (Π and Π^*) orbital concerning the band edges of MoS₂. These results can help find the type of band alignment between MoS₂

and an anthracene molecular crystal, as well as the binding energy of the molecule on the surface. The financial support by DFG within CRC 1242 (*Project B 02*) and computation time on the MagnitUDE supercomputer system are gratefully acknowledged.

O 74.7 Thu 12:00 GER 37

Lateral heterostructures of graphene and h-BN with atomic lattice coherence and tunable rotational order — •HAOJIE GUO¹, ANE GARRO-HERNANDORENA¹, ANTONIO J. MARTÍNEZ-GALERA^{2,3}, and JOSÉ M. GÓMEZ-RODRÍGUEZ^{1,3,4} — ¹Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — ²Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — ³Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — ⁴Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

In-plane heterostructures of graphene and h-BN exhibit exceptional properties, which are sensitive to the structure of the alternating domains. However, achieving accurate control over their structural properties, while keeping a high perfection of the graphene-h-BN boundaries, still remains a challenge. Here, the growth of lateral heterostructures of graphene and h-BN on Rh(110) surfaces is reported. The choice of the 2D material, grown firstly, determines the structural properties of the whole heterostructure layer, allowing to have control over the rotational order of the domains. The atomic-scale observation of the boundaries demonstrates a perfect lateral matching. Lateral heterostructures floating over an oxygen layer have been successfully obtained, enabling to observe intervalley scattering processes in graphene regions. The high tuning capabilities of these heterostructures suggests their usage as testbeds for fundamental studies.

O 74.8 Thu 12:15 GER 37

Relaxation mechanisms for in-plane heterostructures of transition metal dichalcogenide monolayers — •KAI MEHLICH¹,

FRANCIS H. DAVIS³, THAIS CHAGAS¹, DANIELA DOMBROWSKI², DANIEL WEBER¹, CATHERINE GROVER¹, ARKADY KRASHENINNIKOV³, and CARSTEN BUSSE¹ — ¹Department Physik, Universität Siegen, Walter-Flex-Str. 3, 57072 Siegen — ²Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — ³Ion Beam Centre, Helmholtz-Zentrum Dresden Rossendorf, Bautzner Landstraße 400, 01328 Dresden

We use sequential epitaxial growth to synthesise in-plane heterostructures of MoS₂ and TaS₂ monolayers on Au(111). Even though the two materials have significantly different lattice constants, STM-measurements show that coherent interconnection of the two materials can be achieved. Defects at the interface such as dislocations are absent. We find this for all interfaces, independent of orientation or the widths of the joined materials. This is at variance with DFT-calculations where we find that the formation of dislocations is energetically favoured, at least until a critical width of the heterostructures. Our growth process can thus lead to a metastable, defect-free interface.

O 74.9 Thu 12:30 GER 37

Predicting the Gas Sensing Performance of 2D Materials — •UDO SCHWINGENSCHLÖGL, VASUDEO BABAR, HAKKIM VOVUSHA, and ALTYNBEK MURAT — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

We study the potential of material simulations based on first-principles methods to predict gas sensing properties of 2D materials. This emerging class of materials is of particular interest to gas sensing applications due to high surface-to-volume ratios and chemical stability. We discuss results of electron transport calculations within the Landauer-Büttiker formalism and compare the conclusions to analyses in terms of the adsorption energy. Journal References: ACS Appl. Nano Mater. 2, 6076 (2019); J. Phys. Condens. Matter 32, 355602 (2020)