CPP 49: 2D Materials VII: Heterostructures (joint session O/CPP)

Time: Thursday 10:30–12:45 Location: GER 37

CPP 49.1 Thu 10:30 GER 37

In-situ growth characterization of 2D heterostructures: $MoSe_2$ on intercalated graphene/Ru(0001) — •Lars Buss[1], Nicolas Braud[2], Moritz Ewert[1], Matteo Jugovac[3], Tevfik Onur Mentes[3], Andrea Locatelli[3], Jens Falta[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Institute for Solid State Physics, University of Bremen, Bremen, Germany — [3]Elettra-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 $MoSe_2$ 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, $MoSe_2$ has been prepared via co-deposition of Mo and Se. Prior Se intercalation of the graphene appears to enhance the subsequent growth of $MoSe_2$ on the graphene. At elevated temperatures, rotational ordering of the $MoSe_2$ is facilitated by the strongly enhanced mobility of single-domain $MoSe_2$ 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 $MoSe_2$ as well as the free-standing character of the Se-intercalated graphene underneath.

CPP 49.2 Thu 10:45 GER 37

Designer quantum states in metal-organic frameworks — •Orlando J Silveira[1], Linghao Yan[1], Shawulienu Kezilebieke[2], Benjamin Alldritt[1], Viliam Vano[1], Ondřej Krejčí[1], Jose Lado[1], Adam S Foster[1,3], and Peter Liljeroth[1] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]University of Jyväskylä, FI-40014 University of Jyväskylä, Finland — [3]Kanazawa 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 M_2DCA_3, with M= Cu and Ni. The two MOFs have been fabricated either on a graphene/Ir(111) surface or the superconducting substrate $NbSe_2$, 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 Cu_2DCA_3 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 Ni_3DCA_2 MOF has a spin density around the Ni atom when synthesized on the $NbSe_2$ substrate due to charge transfer, and this makes a perfect platform to realize topological superconductivity.

CPP 49.3 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 Boban[5], Lukasz Plucinski[5], Markus Ternes[1,2,4], F. Stefan Tautz[1,2,3], and Felix Lüpke[1,2] — [1]Peter-Grünberg-Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) - 52425 Jülich, Fundamentals of Future Information Technology, Germany — [3]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany — [4]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany — [5]Peter-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.

CPP 49.4 Thu 11:15 GER 37

Fermi level tuning of a $MnBi_2Te_4$ monolayer — •Marco Dittmar[1], Philipp Kagerer[1], Celso I. Fornari[1], Simon Müller[1], Sergio L. Morelhão[2], Hendrik Bentmann[1], and Friedrich Reinert[1] — [1]Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany — [2]Instituto 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 $MnBi_2Te_4$, acting as a magnetic extension of the topological insulator Bi_2Te_3 [1]. We tune the Fermi level position in this compound by preparing a single layer of $MnBi_2Te_4$ on top of the topologically non-trivial p-n-junction of Sb_2Te_3 and Bi_2Te_3 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)

CPP 49.5 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 Samuely[4], Keda Jin[1,2], Oleksander Onufriienko[4], F. Stefan Tautz[1,3,5], Markus Ternes[1,2,3], and Felix Lüpke[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen, Germany. — [3]Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, 52425 Jülich, Germany — [4]Centre of Low Temperature Physics, Faculty of Science, P. J. Safarik University & Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia — [5]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen, Germany

The 2D topological insulator monolayer (ML) WTe_2 is characterized by an insulating interior surrounded by helical 1D edge states. When this material is brought into proximity to the s-wave superconductor $NbSe_2$, 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 WTe_2 and $NbSe_2$, 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)

CPP 49.6 Thu 11:45 GER 37

Density functional theory studies of Anthracene on MoS_2 — •Gérald Kämmerer and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen

Thin layers of MoS_2 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 ($C_{14}H_{10}$) on a MoS_2 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 MoS_2. These results can help find the type of band alignment between MoS_2

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.

CPP 49.7 Thu 12:00 GER 37

Lateral heterostructures of graphene and h-BN with atomic lattice coherence and tunable rotational order — •Haojie Guo[1], Ane Garro-Hernandorena[1], Antonio J. Martínez-Galera[2,3], and José M. Gómez-Rodríguez[1,3,4] — [1]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [4]Condensed 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.

CPP 49.8 Thu 12:15 GER 37

Relaxation mechanisms for in-plane heterostructures of transition metal dichalcogenide monolayers — •Kai Mehlich[1], Francis H. Davis[3], Thais Chagas[1], Daniela Dombrowski[2], Daniel Weber[1], Catherine Grover[1], Arkady Krasheninnikov[3], and Carsten Busse[1] — [1]Derpartment Physik, Universität Siegen, Walter-Flex-Str. 3, 57072 Siegen — [2]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [3]Ion Beam Centre, Helmoltz-Zentrum Dresden Rossendorf, Bautzner Landstraße 400, 01328 Dresden

We use sequential epitaxial growth to synthesise in-plane heterostructures of MoS_2 and TaS_2 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.

CPP 49.9 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)