HL 14: 2D Materials and their Heterostructures II (joint session DS/HL)

Time: Tuesday 9:30–13:00 Location: H3

Invited Talk HL 14.1 Tue 9:30 H3

Graphene-based epitaxial 2D heterosystems: making graphene great again — •Christoph Tegenkamp — Institut für Physik, TU Chemnitz

2D materials and their heterostructures are at the forefront of research, anticipated to serve as fundamental building blocks for new quantum materials. Proximity coupling is a key concept in this domain, enabling diverse and novel functionalities. Epitaxial graphene (EG) grown on SiC(0001) resembles a truly 2D electron gas system, celebrated for its manifold and flexible functionalization schemes at both its vacuum and interface sites. These functionalization strategies enable extreme doping scenarios in graphene, tuning spin-orbit coupling, realizing interface states, or introducing mini-bands through zone folding. The controlled transition from linear to flat bands in EG, along with the coupling of functionalized epitaxial graphene to 2D electron gases (2DEGs), opens avenues for exploring electronic correlation effects and mesoscopic phenomena in epitaxial 2D heterostructures. In this presentation, I will showcase some recent findings achieved through the adsorption and intercalation of elements such as Pb and Sn, demonstrating their potential to further tune the properties of graphene.

HL 14.2 Tue 10:00 H3

Proximity-induced spin-orbit coupling in bilayer graphene quantum wires — •Michael Laumer and Angelika Knothe — Universität Regensburg, 93053 Regensburg, Germany

The gate-tuneable band gap and the possibility to tailor its band structure by proximitizing with other 2D materials [1] make bilayer graphene (BLG) an excellent platform for future quantum technologies. By applying spatially modulated displacement fields, one may confine BLG's charge carriers into electrostatically induced nanostructures [2, 3]. Proximitizing the BLG with a transition metal dichalcogenide (TMDC) strongly enhances the SOC of the adjoining graphene layer [1]. Fascinated by the concept of proximity-tailoring BLG nanostructures, we convey the idea of proximity-inducing SOC to a gate-confined BLG quantum wire. We theoretically study the resulting quantized subband structure for different SOC strengths and as a function of the wire geometry. Our results help us understand how proximity-induced SOC manifests in confined geometries and identify different regimes of the wires' electronic properties.

[1] K. Zollner, M. Gmitra, and J. Fabian. Swapping exchange and spin-orbit coupling in 2d van der waals heterostructures. Phys. Rev. Lett., 125:196402, (2020). [2] A. Knothe and V. Fal'ko. Influence of minivalleys and berry curvature on electrostatically induced quantum wires in gapped bilayer graphene. Phys. Rev. B, 98:155435, (2018). [3] H. Overweg et al. Topologically nontrivial valley states in bilayer graphene quantum point contacts. Phys. Rev. Lett., 121:257702, (2018).

HL 14.3 Tue 10:15 H3

Above room temperature ferromagnetism in large-area Fe_3GaTe_2/graphene van der Waals heterostructures — •Tauqir Shinwari[1], Kacho Imtiyaz Ali Khan[1], Hua Lv[1], Atekelta Abebe Kassa[1], Frans Munnik[2], Achim Trampert[1], Michael Hanke[1], Jens Herfort[1], and Joao Marcelo Jordao Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V. Dresden, Germany

Two-dimensional (2D) magnetic materials and van der Waals (vdW) heterostructures offer new possibilities for the realization of advanced spintronic devices. Fe_3GaTe_2, a 2D ferromagnetic metal with a high Curie temperature ($\sim$ 360K) and strong perpendicular magnetic anisotropy, has emerged as a promising candidate for energy-efficient magnetic devices. However, all investigations conducted in Fe_3GaTe_2 so far have been performed using millimeter-sized bulk crystals and flakes exfoliated from them, both not suitable for integration in device processing. Hence, it is crucial to develop controlled large-scale growth of this material and investigate its properties. In this contribution, we present a breakthrough in the high-quality, large-area epitaxial growth of Fe_3GaTe_2 thin films on epitaxial graphene/SiC(0001) substrates using molecular beam epitaxy. These results are highly relevant for the future development of high-performance spintronic devices based on 2D heterostructures potentially revolutionizing data storage, processing, and quantum computing applications.

HL 14.4 Tue 10:30 H3

Modeling carbon nanomembranes through molecular dynamics simulations — •Levin Mihlan and Jürgen Schnack — University of Bielefeld

Carbon nanomembranes (CNMs) are nanometer-thin materials synthesized via electron-induced crosslinking of aromatic self-assembled monolayers. CNMs can be functionalized for various applications, initially serving as molecular filters. Due to their presumed irregular internal structure, these membranes pose challenges for standard spectroscopic efforts, often being insufficiently informative [1]. Ehrens et al. initially conducted molecular dynamics simulations to investigate CNM formation, replicating crosslinking and pore formation via momentum transfers in carbon-only systems [2]. Here, we extend the approach by incorporating hydrogen atoms, which may play a critical role in the crosslinking process, even though they largely disappear in the final CNM products. This additionally reduces the number of theoretical assumptions. We examine whether and in what way pores form and analyze properties such as aromaticity, sp content, and Young's modulus to compare with previous simulations and experiments.

[1] Dementyev, Petr, et al. "Carbon Nanomembranes from Aromatic Carboxylate Precursors" Chem. Phys. Chem 21, 1006 (2020)
[2] Ehrens, Julian, et al. "Theoretical formation of carbon nanomembranes under realistic conditions using classical molecular dynamics" Phys. Rev. B 103, 115416 (2021)

session break

HL 14.5 Tue 11:00 H3

Photo-electrochemical oxidation and thinning of transition metal dichalcogenides — •Simon Wörle[1], Lukas Wolz[1], Franz Gröbmeyer[2], Emiliano Cortes[2], Jeremy Robinson[3], and Ian Sharp[1] — [1]Walter Schottky Institute, Physics Department and TUM School of Natural Science, Technical University of Munich — [2]Nanoinstitute Munich and Faculty of Physics, Ludwig-Maximilians-Universität — [3]Naval Research Laboratory, Washington, D.C

Two-dimensional transition metal dichalcogenides (TMDs) exhibit unique optoelectronic and mechanical properties. For their integration in functional devices and for catalytic applications, it is crucial to understand and control their behavior in the reactive environments. Here, we investigate the stability of thin MoS_2, WS_2, $MoSe_2$ and WSe_2 films in acidic, neutral, and basic solutions using a three-electrode photoelectrochemical cell, which enables experiments under both illumination and in the dark. Under anodic conditions, sulfides and selenides undergo different protonic reactions, depending on the pH of the electrolyte, resulting in different resistances to oxidation. Additional exposure to light from a solar simulator creates photo-excited holes, which drive a self-limiting electrochemical thinning procedure that enables the top-down fabrication of large-area TMDs with a thickness of only a few layers. The degradation, initiated at the edges or defects, propagates through the flakes and can be monitored in-situ using an optical microscope. Under laser excitation, multilayer TMDs can be thinned in predefined patterns, paving a new route for processing and integration of 2D materials into functional devices.

HL 14.6 Tue 11:15 H3

Rapid MOCVD synthesis of stratified MoS2 and WS2 2D heterostructures — •Nikolas Dominik, Sebastian Klenk, Cormac Ó Coileáin, and Georg S. Duesberg — Institute of Physics, University of the Bundeswehr Munich & SENS Research Center, München, Deutschland

The two-dimensional (2D) structure of layered materials such as the transition metal dichalcogenides MoS2 and WS2, imparts exceptional electrical, mechanical and optical properties. This makes them particularly interesting for electronic, photovoltaic and sensing application. Van der Waals heterostacks, composed of assembled 2D materials, expand on the possible range of properties, and so have attracted extensive attention due to factors such as ultrafast carrier transport and high bandgap tunability.

Here we present metal-organic chemical vapour deposition (MOCVD) synthesis of MoS2/WS2 combination heterostructures us-

ing a highly controllable industrial-scale multi-precursor system, thus avoiding the laborious need for manual stacking. We show how this synthesis method allows the creation of clearly defined and highly ordered stacks by producing a 7-layer combination structure below 10 nm. We explore the characteristics of these films using Raman spectroscopy and XPS, EDX, TOF-SIMS and microscopy techniques.

HL 14.7 Tue 11:30 H3

Unveiling the mechanism of monolayer selective large-area exfoliation of 2D materials — •Jakob Ziewer[1], Abyay Ghosh[1], Michaela Hanušová[2], Luka Pirker[2], Otakar Frank[2], Matěj Velický[2], Myrta Grüning[1], and Fumin Huang[1] — [1]Queen's University Belfast, Belfast, U.K. — [2]J. Heyrovský Institute of Physical Chemistry

Metal assisted exfoliation has made it possible to selectively isolate single crystal monolayers of 2D materials at sizes up to a centimetre [1][2]. This represents a million fold increase compared to standard tape exfoliation.

In this presentation the mechanism of enhanced yield is discussed. Through spectroscopic measurements and observation of macroscopic bubbles it is discovered that the Au substrate decouples attached MoS_2 monolayers from the remaining crystal. The interfacial weakening is dependant on the thickness of the crystal and is maximised for thick crystals.

These findings are used to explain the mechanism behind metal assisted exfoliation and are expected to extend to other Au-2D heterostructures.

[1] Velický, M.; et. al. Mechanism of Gold-Assisted Exfoliation of Centimeter-Sized Transition-Metal Dichalcogenide Monolayers. ACS Nano 2018, 12, 10463*10472. [2] Huang, Y.; et. al. Universal Mechanical Exfoliation of Large-Area 2D Crystals. Nat. Commun. 2020, 11:2453.

session break

HL 14.8 Tue 12:00 H3

Probing the electronic band structure of the 2D magnetic materials MPS3 (M=Fe,Ni) across magnetic phase transitions — •Jeff Strasdas[1], Benjamin Pestka[1], Biplab Bhattacharyya[1], Adam K. Budniak[2], Marcus Liebmann[1], Niklas Leuth[1], Honey Boban[3], Lutz Waldecker[1], Bernd Beschoten[1], Christoph Stampfer[1], Lukasz Plucinski[3], Efrat Lifshitz[2], and Markus Morgenstern[1] — [1]II. Inst. Phys. B and JARA-FIT, RWTH, Aachen, Germany — [2]Schulich Chem. Fac., Solid State Inst., Russell Berrie Nanotech. Inst., Helen Diller Quantum Center, Technion - Israel Inst. of Technology, Haifa, Israel — [3]Forschungszentrum Jülich, Peter Grünberg Inst. (PGI-6), Jülich, Germany

We investigate the band structure of the van der Waals materials FePS3 [1] and NiPS3, both 2D antiferromagnetic insulators, using μm-scale Angular Resolved Photoelectron Spectroscopy (ARPES), above and below their Néel temperatures (TN). The data is compared with DFT+U calculations and simplified selection rules to deduce the orbital character of changing bands. In FePS3, we observe three distinct band structure changes across TN, involving bands with Fe 3d, S 3p, and pure P 3p character, reflecting the intricate competition of direct exchange between Fe atoms and superexchange via S and P atoms. In NiPS3, we identify one band shift near Γ across TN, containing a band of mixed Ni and S character. Here, pronounced deviations from the DFT+U calculations indicate more complex electronic correlations. Moreover, we refine the photoelectron selection rules using ARPES data from CrPS4. [1] B. Pestka et al. doi:10.1021/acsnano.4c12520

HL 14.9 Tue 12:15 H3

Investigation of 1T-TaS2 phase transition and charge transfer phenomena at interfaces with perovskites — •Georgios Chatzigiannakis[1,2], Anastasia Soultati[1], Spiros Gardelis[2], and Maria Vasilopoulou[1] — [1]Institute of Nanoscience and Nanotechnology, National Centre of Scientific Research Demokritos, 15341 Athens, Greece — [2]Department of Physics, National and Kapodistrian University of Athens, 15784 Athens, Greece

1T-TaS2 is a distinguished 2D-layered transition metal dichalcogenide with a rich phase diagram upon cooling including charge density wave (CDW) states and a Mott insulating phase. On the other hand, halide perovskites (HPs) are emerging as a unique class of materials in the field of photonics due to their intriguing optoelectronic properties. The combination of 1T-TaS2 with HPs is proposed as a viable solution to overcome the drawbacks of each category thanks to charge transfer phenomena.

In this work, we studied the phase transitions of 1T-TaS2 as a function of the cooling rate. In the case of nanothick crystals, CDW phase transitions were observed upon gradual cooling but they were totally absent afrer a vigorous cooling. On the contrary, for bulk crystals the CDW phase transitions were totally independent of the cooling rate. Furthermore, we developed 1T-TaS2/HPs heterostructures and we investigated charge transfer phenomena by XPS and UPS spectroscopy, both revealing electron transfer from 1T-TaS2 towards perovskite. Charge transfer could also enable the development of high-performance hybrid optoelectronic devices based on these materials.

HL 14.10 Tue 12:30 H3

The effect of a perpendicular electric field on charge-spin interconversion coefficients in proximitized graphene on 1T-TaS_2 monolayer — •Juraj Mnich[1], Marko Milivojević[2,3], and Martin Gmitra[1,4] — [1]Institute of Physics, P.J.Šafárik University in Košice, 04001 Košice, Slovakia — [2]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [3]Institute of Informatics, SAS, 84507 Bratislava, Slovakia — [4]Institute of Experimental Physics, SAS, 04001 Košice, Slovakia

The proximity-induced spin-orbit coupling and exchange interactions in the graphene-based heterostructures provides an effective way to manipulate with charge-spin interconversion coefficients. In the talk we focused on charge-spin interconversion in bilayer and trilayer heterostructures of 1T-TaS_2 and graphene. By modulating the temperature, we can access the charge density wave phase and switch between the magnetic and non-magnetic phases of 1T-TaS_2 affecting consequently the graphene electrons. Using linear response theory we showed the dependence of charge-spin interconversion coefficients on a perpendicular applied electric field. For the specific configurations of the 1T-TaS_2 and graphene we observed a change in both the sign and the magnitude of the non-equilibrium spin density as a response to the perpendicular electric field. This result indicates a possibility of using electric fields as a tool to control the direction of spin density.

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HL 14.11 Tue 12:45 H3

Self spin-orbit torque in proximitized graphene on 1T-TaS_2 monolayer — •Martin Gmitra[1,4], Maedeh Rassekh[1], Juraj Mnich[1], and Marko Milivojević[2,3] — [1]Institute of Physics, P.J.Šafárik University in Košice, 04001 Košice, Slovakia — [2]Faculty of Physics, University of Belgrade, 11001 Belgrade, Serbia — [3]Institute of Informatics, SAS, 84507 Bratislava, Slovakia — [4]Institute of Experimental Physics, SAS, 04001 Košice, Slovakia

We show that self spin-orbit torque induced in graphene-based van der Waals heterostructures represents a platform to extract the Rashba phase – a proximity-induced spin-orbit coupling parameter. Performing first-principles calculations, tight-binding modeling, and non-equilibrium Greens function transport calculations for graphene on 1T-TaS_2 monolayer we found that charge current in graphene generates non-equilibrium spin accumulation and self-torque in graphene due to the proximity-induced spin-orbit coupling and exchange interaction. The Rashba spin-orbit torque is a dominant contribution and weakly depends on the direction of magnetization in 1T-TaS_2. We propose that the magneto-optical Kerr effect can directly extract the Rashba spin-orbit coupling phase.

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