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

Time: Wednesday 15:00–17:30 Location: REC/C213

DS 14.1 Wed 15:00 REC/C213

Engineering at the Thinnest Scale: Insights into the Stability of 2D GaN on Liquid Metal Catalysts — •Tomoko Yokaichiya, Karsten Reuter, and Hendrik H. Heenen — Fritz-Haber-Institut der MPG, Berlin

Hexagonal GaN (h-GaN), theorized to be metastable when confined to only a few nanometers, stands out as a promising wide-bandgap semiconductor for next-generation nanoelectronics. Although early studies report that h-GaN can be synthesized using e.g. liquid metal catalysts, its definitive experimental identification is challenging. This difficulty arises from a structural ambiguity due to possible defects, multilayer-stacking variations, and competing polymorphs of h-GaN's characteristic honeycomb structure, as predicted by pioneering, yet simplified electronic-structure studies. In this work, we use density functional theory alongside large-scale atomistic simulations based on machine-learned interatomic potentials to re-assess the stability of h-GaN at finite temperatures and in the presence of a liquid metal substrate. We systematically investigate the structural and electronic properties of h-GaN, examining how they evolve with layer thickness and possible structural variations. Furthermore, we analyze its thermodynamic competition with bulk wurtzite GaN and alternative thin-film polymorphs, including a previously suggested haeckelite phase. Our results reveal that h-GaN exists within a delicate stability window. Based on these insights, we propose key signatures to guide experimental detection and outline whether h-GaN may become synthesizable as a feasible 2D semiconductor.

DS 14.2 Wed 15:15 REC/C213

Superconducting and dielectric properties of monolayer α-$TaSi_2N_4$ — •Timon Mosko[1] and Martin Gmitra[1,2] — [1]Institute of Physics, Pavol Jozef Safarik University in Kosice, Park Angelinum 9, 04001 Kosice, Slovakia — [2]Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 04001 Kosice, Slovakia

The monolayer α-$TaSi_2N_4$ belongs to the recently discovered MA_2Z_4 family of two-dimensional intercalated materials, exhibiting wide range of physical properties, including semiconducting, metallic, topological, and superconducting behavior. Members of this group, such as $MoSi_2N_4$, WSi_2N_4 have already been successfully synthesized, highlighting the structural and electronic tunability of the inspected group of materials. We investigated the superconducting and dielectric properties of monolayer α-$TaSi_2N_4$ using a combination of ab initio and effective model approaches. The phonon-mediated superconductivity is examined through first-principles calculations, an effective tight-binding Hamiltonian in Wannier basis and further analyzed within the Migda-Eliashberg theory of superconductivity. Our results reveal that α-$TaSi_2N_4$ is an anisotropic two-band superconductor. Additionally, we study the dielectric response via electric susceptibility using linear response theory within the RPA, combining Green's function formalism with tight-binding modeling.

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DS 14.3 Wed 15:30 REC/C213

Probing the Quantum Spin Hall State in Atomic Monolayers via NanoARPES — •Cedric Schmitt[1,2], Lukas Gehrig[1,2], Kilian Strauss[1,2], Jonas Erhardt[1,2], Matthew Watson[3], Jörg Schäfer[1,2], Simon Moser[1,2,4], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Diamond Light Source, UK — [4]AG Oberflächen, Ruhr-Universität Bochum

Our recently discovered quantum spin Hall insulator indenene [1], a triangular monolayer of indium on SiC(0001), exhibits a 120 meV gap and monodomain growth on the μm scale. To verify its topological nature, we use circular dichroism in ARPES as a bulk-sensitive probe of orbital angular momentum (OAM) linked to its Berry curvature [2]. Due to SiC's stepped morphology, stacking-dependent OAM cancellation complicates microARPES. We overcome this challenge using nanoARPES with sub-600 nm resolution, resolving OAM asymmetry at individual terraces of SiC. Our study establishes dichroism as a robust spectroscopic tool for topological classification within a single SiC terrace.

[1] M. Bauernfeind et al. Nat. Commun. 12, 5396 (2021)
[2] J. Erhardt et al. Phys. Rev. Lett. 132, 196401 (2024)

DS 14.4 Wed 15:45 REC/C213

Physical Properties of $Ti_3C_2Cl_2$ MXenes — •Moritz Vanselow[1], Maksim Riabov[2], Thierry Ouisse[2], Hanna Pazniak[2], and Ulf Wiedwald[1] — [1]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen — [2]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, France

Hydrophobic $Ti_3C_2Cl_2$ MXenes are synthesized by Lewis acid molten-salt etching of $Ti_3C_2Cl_2$ followed by delamination process[1] and subsequently deposited from acetonitrile suspension ($\sim$ 0.1 mg/mL) on $Si(100)/SiO_2$ substrates. Using in-situ mass spectrometry and Auger electron spectroscopy in ultrahigh vacuum, we show that $Ti_3C_2Cl_2$ exhibits enhanced thermal robustness up to 900°C as compared to conventional mixed-terminated $Ti_3C_2T_x$ MXenes with $T_x = -F, = O$, and $-OH$. Complementary ex situ XRD and XPS confirm the absence of intercalated water and uniform $-Cl$ terminations, resulting in sharp and intense (00l) peaks with $c = 2.223 \pm 0.015$ nm and reflecting its high degree of structural order. Low-temperature specific heat measurements reveal distinct phonon signatures expected for the two-dimensional $Ti_3C_2Cl_2$. We determined the Debye temperature to 548 K in a temperature interval 20–50 K consistent with DFT model calculations[2] and a Sommerfeld constant of $\gamma = 19.2\,\mathrm{mJ\,mol^{-1}\,K^{-2}}$. This work is supported by ANR-23-CE09-0031-01 and DFG ID 530103526.

[1] T. Zhang et al., Chem. Mater. 36, 1998 (2024). [2] M. Riabov, M. Vanselow, et al., npj 2D Materials & Applications 2025, accepted

DS 14.5 Wed 16:00 REC/C213

Phase field crystal model of out-of-plane deformations in thin crystalline sheets induced by thermal expansion — •Emma Radice[1], Marco Salvalaglio[1,2], and Axel Voigt[1] — [1]Institut für Wissenschaftliches Rechnen, Technische Universität Dresden, Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany

Thin, flexible crystalline sheets exhibit unique elastic properties due to their ability to undergo out-of-plane deformations.Understanding this behavior requires a description that couples in-plane elasticity, out-of-plane bending and the presence of defects. We develop a mesoscale description for these systems by extending the Phase-Field Crystal (PFC) model. PFC model describes crystal structures at diffusive timescales through a periodic, microscopic density field and it allows one to incorporate both elasticity and topological defects into a continuum description. Our extension permits a spatially varying equilibrium lattice spacing, enabling the representation of localized lattice eigenstrain to mimick thermal effects or lattice mismatch in heterostructures. We validate the extended model against analytical predictions from the Föppl von Kármán equations for uniaxial compression and from Eshelby's inclusion problem. Using this validated framework, we then study how locally induced compressive stresses drive out-of-plane deformation (buckling) in the sheets. Our approach, implemented via a Fourier pseudo-spectral method, exploits the PFC model's natural ability to capture the complex, coupled interactions among elasticity, out-of-plane bending and defect dynamics.

15 min. break

DS 14.6 Wed 16:30 REC/C213

Magnetotransport in Z-Folded ABC-Stacked Trilayer Graphene Structures — •Maximilian Mischke, Lina Bockhorn, Sofiya Lazareva, and Rolf Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

Folded graphene (multi)layers promise to contain rich and interesting physics [1-3], so we produced a sample to investigate the influence of such a fold on magnetotransport properties of graphene. The measurements were carried out in a 4He cryostate at 1.4 K while the samples' carrier concentration was controlled via a global backgate. The sample itself consists of a z-folded ABC-trilayer graphene partially encapsulated in hBN with electrical contacts that allow for measurements in the unfolded region as well as through the fold. We observed filling

factors that are unexpected for ABC-trilayer graphene. The untypical transport behaviour can be explained by angle dependend interlayer coupling and screening effects in the z-fold.

[1] S. J. Hong et al, Phys Rev B 105, 205404 (2022)
[2] H. Schmidt et al, Nature Communications 5(1), 5742 (2014)
[3] Y. Liu et al, Phys Rev B 92, 235438 (2015)

DS 14.7 Wed 16:45 REC/C213

Quantum dots in proximitized BLG/TMD heterostructures — •Ching-Hung Chiu and Angelika Knothe — Institut für Theoretische Physik, Universität Regensburg, 93053 Regensburg, Germany

Bilayer graphene (BLG) has attracted attention recently due to the possibility of inducing layer-selective Spin-orbit coupling (SOC) by proximitizing with transition metal dichalcogenides (TMDs) [1,2]. Simultaneously, the gate-tunable band gap in BLG enables electrostatic confinement of charge carriers into gate-defined quantum point contacts and quantum dots [3,4]. Here, we theoretically investigate the interplay of proximity effects and confinement by studying confined quantum states in proximitized BLG/TMD quantum dots. We calculate the states' properties, such as their splittings and spin polarisation, as a function of SOC coupling parameters and the dot's size and shape. Our studies go alongside experimental realisations of confinement in BLG/TMD heterostructures [5,6] and pave the way for using and controlling the dot's spin and valley states as qubits.

[1] K. Zollner and J. Fabian, Phys. Rev. B 104, 075126 (2021)
[2] A. M. Seiler et al., 2025 2D Mater. 12 035009
[3] H. Overweg et al., Phys. Rev. Lett. 121, 257702 (2018)
[4] S. Möller et al., Phys. Rev. Lett. 127, 256802 (2021)
[5] J. D. Gerber et al., Nano Lett. 2025, 25, 33, 12480-12486
[6] H. Dulisch et al., Nano Lett. 2025, 25, 26, 10549-10555

DS 14.8 Wed 17:00 REC/C213

Influence of Polymethyl Methacrylate molecular weight on Graphene transfer and its intrinsic properties — •Monika Choudhary[1], Rasuole Lukose[1], Moriom Akter[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]Leibniz-Institut für Innovative Mikroelektronik (IHP), Frankfurt Oder, Germany — [2]Semiconductor Materials, BTU Cottbus-Senftenberg, Cottbus, Germany

Polymethyl methacrylate (PMMA)-assisted wet transfer is widely used for integrating large-scale graphene grown on Ge(100)/Si substrates via chemical vapor deposition onto insulating SiO2/Si substrates[1,2]. However, the influence of PMMA molecular weight (MW) on properties of transferred graphene is insufficiently quantified. To address this, we investigate graphene transferred using low (50K), medium (600K), and high (950K) MW PMMA to isolate how polymer chain length governs film integrity and contamination. Characterization by atomic force microscopy (AFM), and spatially resolved X-ray photoelectron spectroscopy (XPS) reveals reduced contamination and smoother topography for graphene with 600K transfers. Additionally, micro-Raman spectroscopy demonstrates strain-free graphene with reduced doping and a 2D peak full width at half maximum (FWHM) of 35.53 cm-1 consistent with as-grown values. 1. Akhtar F., et al. ACS Appl. Mater. Interfaces 15 (2023). 2. Lukose R., et al. Scientific Reports 11 (2021). Acknowledgement: This research was funded by the European Union*s Horizon Europe research and innovation programme under grant agreement No 101120938 (GATEPOST).

DS 14.9 Wed 17:15 REC/C213

High-performance graphene field-effect transistors on cyclic olefin copolymer substrates for advanced sensor applications — •Hamid Reza Rasouli[1], Begimai Adilbekova[1], Ghazaleh Eshaghi[1], Axel Printschler[1], David Kaiser[1], Marco Reinhard[2], Alexander Rolapp[2], Tom Reinhold[2], Uwe Hübner[3], Michael Meister[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]IMMS Institut für Mikroelektronik- und Mechatronik-Systeme gemeinnützige GmbH (IMMS GmbH), 99099 Erfurt, Germany — [3]Leibniz Institute of Photonic Technology, Albert-Einstein-Straße 9, 07745 Jena, Germany

While graphene field-effect transistors (GFETs) are highly attractive for liquid-phase sensing, their performance on SiO2/Si substrates is compromised by oxide-induced charge trapping, leading to pronounced hysteresis and reduced stability. We present arrays of GFETs microfabricated on cyclic olefin copolymer (COC) substrates, which passivate SiO2 providing a low-trap and chemically inert platform in combination with flatness. GFET devices on COC demonstrate remarkably improved Dirac point stability, negligible hysteresis even in low-ionic strength buffers, and reproducibility across the arrays. For their functionalization, we employ an ultrathin carbon nanomembrane (CNM) that enables robust immobilization of various capture molecules while preserving graphene's transport properties. The CNM/GFET/COC architecture provides stable liquid-phase operation highlighting its strong potential for scalable and advanced sensor applications.