DS 3: 2D Materials and their Heterostructures I (joint session DS/HL)

Time: Monday 15:00–17:45 Location: H3

DS 3.1 Mon 15:00 H3

Nanoscale NMR of two-dimensional solids using NV centers in diamond — •Marcel Martin[1], Mokessh Kannah Ciwan[1], Yejin Lee[2], Jakob Nachtigal[1], Nicola Poccia[3,4], Uri Vool[2], Jürgen Haase[1], and Nabeel Aslam[1] — [1]Leipzig University, Leipzig, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [4]Department of Physics, University of Naples Federico II, Naples, Italy

Nuclear magnetic resonance (NMR) is a powerful method to investigate electronic properties of condensed matter but is inherently limited by its low sensitivity. Nitrogen-vacancy (NV) centers in diamond are quantum sensors that allow extending NMR to thin films and μm-scale exfoliated flakes of 2D materials which exhibit electronic phases such as charge density waves (CDW) and superconductivity. For the latter, NMR is especially powerful as it can elucidate the pairing symmetry of the charge carriers.
In this talk, we first discuss solid-state nano-NMR with NV centers of CaF_2, a testbed material for this method. The ultimate goal, however, is to study the CDW and Ising superconductivity phases of few-layer NbSe2 with nano-NMR. In this context, we present initial optical studies of $NbSe_2$ flakes which have been exfoliated and transferred onto a diamond. In addition to this, we will present results of conventional NMR on bulk $NbSe_2$ which serve as a reference.

DS 3.2 Mon 15:15 H3

Twist-tunable spin control in twisted bilayer bismuthene — •Ludovica Zullo[1,2,3,4], Domenico Ninno[4,5], and Giovanni Cantele[5] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy — [3]Sorbonne Université, CNRS, Institut des Nanosciences de Paris, UMR7588, F-75252 Paris, France — [4]Dipartimento di Fisica E. Pancini, Università degli Studi di Napoli *Federico II*, Complesso Universitario M. S. Angelo, via Cintia 21, 80126, Napoli, Italy — [5]CNR-SPIN, c/o Complesso Universitario M. S. Angelo, via Cintia 21, 80126, Napoli, Italy

The role of spin-orbit coupling (SOC) in twisted bilayers has gained increasing attention due to its potential for spintronics, opening a quest for new layers with substantial SOC. In this work [1], by means of first principles calculations, we investigate how the interplay between SOC and twist angle impacts the band structure and spin textures of twisted bilayer bismuthene. We find that the twist angle can be deemed a control knob to switch from a small-gap semiconductor to a metallic behavior. Most crucially, the accurate analysis of the energy bands close to Fermi energy reveals a twist-tunable splitting in the mexican-hat shape of the bands that can otherwise be obtained only by applying enormous electric fields, providing insight into innovative technologies for future spintronic devices. [1] Ludovica Zullo, Domenico Ninno, Giovanni Cantele, Phys. Rev. B, 110, 165411 (2024)

DS 3.3 Mon 15:30 H3

Iron Diffusion in Thermally Stable $Ti_3C_2Cl_2$ MXenes under UHV Conditions — •Moritz Vanselow[1], Maksim Riabov[2], Hanna Pazniak[2], Thierry Ouisse[2], and Ulf Wiedwald[1] — [1]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen, Germany — [2]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, France

MXenes are 2D materials derived from a MAX phase precursor. Molten salt etching of $Ti_3C_2Cl_2$ results in hydrophobic $Ti_3C_2T_X$ MXenes with T_X = -Cl as a termination species [1]. $Ti_3C_2Cl_2$ MXenes are deposited on $Si(100)/SiO_2$ and we in situ study its chemical stability by mass spectrometry and Auger electron spectroscopy in ultrahigh vacuum. Compared with standard hydrophilic $Ti_3C_2T_X$ MXenes, where T_X = -F, =O, and -OH, fluorine and hydroxyl groups can be removed by annealing at temperatures up to 1000 K, the thermal stability of $Ti_3C_2Cl_2$ MXenes is significantly enhanced. Moreover, intercalated water changing the MXene sheet separation, is not present in hydrophobic $Ti_3C_2Cl_2$ as proven by ex situ X-ray diffraction, wide-angle X-ray scattering (WAXS) and X-ray photoelectron spectroscopy (XPS). After optimizing the annealing procedure, we in situ intercalate Fe by e-beam assisted deposition on top of MXene thin films and subsequent Fe diffusion by soft annealing at 600 K. This work is funded by a joint ANR-DFG-Project under ANR-23-CE09-0031-01 and DFG ID 530103526. [1] T. Zhang et al., Chem. Mater. 36, 1998 (2024).

DS 3.4 Mon 15:45 H3

Interactions Between Two-Dimensional Crystals and Molecules via Density Functional Theory — •Stefan Wolff[1], Xin Chen[2], Tobias Dierke[1], and Janina Maultzsch[1] — [1]Department of Physics, Chair of Experimental Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Institute of Chemistry and Biochemistry, Freie Universität Berlin

The unique properties of two-dimensional (2D) materials can be modified through chemical functionalization, driven by their interactions with functional groups or molecules. Density functional theory (DFT) calculations are employed to investigate non-covalent functionalization of bilayer graphene with 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN) molecules. The interactions between the graphene layers and the HATCN molecules play a significant role in determining the functionalization behavior, which depends on the stacking arrangement. Locally stacked regions within the moiré lattice of twisted bilayer graphene (tBLG) play a crucial role for functionalization. Consequently, the moiré pattern of tBLG can serve as a template to control the degree of functionalization. Furthermore, laser-triggered covalent functionalization of molybdenum disulfide (MoS_2) enables the fabrication of patterned 2D heterostructures with phenyl-based interface linkers. Through DFT calculations, various potential binding motifs and their associated optical properties are predicted. Calculations of reaction energies and Raman modes provide insights into the likelihood of different reaction pathways and the structures they yield.

DS 3.5 Mon 16:00 H3

Toward high-sensitivity and low-power consumption gas sensor devices based on 2D-transistors. — •Aurelio García Valenzuela[1], Zahra Fekri[1], Madhuri Chennur[1], Nikol Lambeva[1], Jens Zscharschuch[1], Victoria Constance Köst[2], Krysztof Nieweglowski[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [2]Institute of Electronic Packaging Technology, AVT, TU-Dresden, Germany

Two-dimensional (2D) materials exhibit excellent properties compared to their bulk counterparts and are promising for applications like gas sensors. Their high surface-to-volume ratio and surface-active sites enhance gas absorption and sensitivity, addressing challenges in detecting low concentrations and reducing power consumption.

This work presents the fabrication and testing of 2D materials-based field-effect transistor (FET) gas sensors. Mechanically exfoliated 2D materials are stacked into heterostructures to create back-gated FETs, with device patterning achieved via electron beam lithography.

The devices were exposed to NH3 and NO2 gases at various temperatures. Gas interactions caused systematic changes in p- and n-type currents and shifts in the transfer curve, depending on gas concentration and type (donor or acceptor). These results demonstrate the suitability of 2D materials-based FETs as efficient and sensitive gas sensors.

short break

DS 3.6 Mon 16:30 H3

Pressure-dependent Effective Hamiltonian and Topological Transitions for Twisted Bilayer Transition Metal Dichalcogenides — •Miftah Hadi Syahputra Anfa[1], Sabri Elatresh[1,2], Hocine Bahlouli[1,3], and Michael Vogl[1,2] — [1]Physics Department, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia — [2]Interdisciplinary Research Center (IRC) for Intelligent Secure Systems, KFUPM, Dhahran, Saudi Arabia — [3]Interdisciplinary Research Center (IRC) for Advanced Materials, KFUPM, Dhahran, Saudi Arabia

Recent studies have shown the existence of nontrivial topological moire bands in twisted bilayer transition metal dichalcogenides (TMDs), which depend on the twist angle. Motivated by this, we present a

study of such a system under applied vertical pressure. The study begins by first considering the untwisted bilayer case without pressure. We find that the system can be described by an effective low-energy Hamiltonian that behaves approximately quadratic and includes layer-shift dependent terms that we were able to determine by symmetry. The structure is then relaxed under pressure in the 0.0 - 3.5 GPa range using ab initio density functional theory (DFT). The DFT band structures for each corresponding pressure are fitted to the effective Hamiltonian to obtain the pressure-dependent parameters. Consecutively, the explicit expression for the twisted pressure-dependent Hamiltonian is obtained by treating the twist as a position-dependent shift between layers. We then present changes in Chern number results for the important energy bands due to pressure.

DS 3.7 Mon 16:45 H3

Effect of spin-dependent tunneling in a $MoSe_2/Cr_2Ge_2Te_6$ van der Waals heterostructure on exciton and trion emission — •Annika Bergmann[1], Swarup Deb[1,2], Veronika Schneidt[1], Mustafa Hemaid[1], Kenji Watanabe[3], Takashi Taniguchi[4], Rico Schwartz[1], and Tobias Korn[1] — [1]Institute of Physics, Rostock University, Rostock, Germany — [2]Saha Institute of Nuclear Physics, Kolkata, India — [3]Research Center for Electronic and Optical Materials, Tsukuba, Japan — [4]Research Center for Materials Nanoarchitectonics, Tsukuba, Japan

In recent years, thin films of magnetic van der Waals materials have gained increasing interest due to their potential applications in spintronics. For instance, heterostructures (HS) consisting of ferromagnetic CRI_3 and a WSe_2 monolayer have demonstrated the existence of magnetic proximity effects, manifesting in the lifting of WSe_2 valley degeneracy as well as helicity-dependent photoluminescence (PL) emission of the WSe_2 monolayer in proximity to the 2D ferromagnet [1,2]. Here, we study HS consisting of monolayer $MoSe_2$ and few-layer ferromagnetic $Cr_2Ge_2Te_6$ (CGT). Under circularly polarized excitation, PL measurements show that the $MoSe_2$ exciton-trion emission ratio depends on the relative orientation of excitation helicity and CGT magnetization, even though the PL emission itself is unpolarized. This hints at an ultrafast, spin-dependent interlayer charge transfer that competes with exciton and trion formation and recombination.

[1] D. Zhong et al., Science Advances, 3 (2017)
[2] D. Zhong et al., Nat. Nanotechnol. 15 (2020)

DS 3.8 Mon 17:00 H3

Magnetic and transport properties of all-epitaxial $Fe_{5-x}GeTe_2/WSe_2$ van der Waals heterostructures — •Hua Lv[1], Tauqir Shinwari[1], Kacho I. A. Khan[1], Jens Herfort[1], Michael Hanke[1], Chen Chen[2], Joan M. Redwing[2], Achim Trampert[1], Mehak Loyal[3], Gerhard Jakob[3], Mathias Kläui[3], Roman Engel-Herbert[1], and João Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]2D Crystal Consortium Materials Innovation Platform, Materials Research Institute, The Pennsylvania State University, PA, United States — [3]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany

Van der Waals (vdW) heterostructures consisting of two-dimensional (2D) ferromagnetic and nonmagnetic materials hold great promises for tailoring their magnetic and transport properties. Here we report on the magnetic and transport properties of all-epitaxial $Fe_{5-x}GeTe_2$ (FGT, with x ≈ 0.2)/WSe_2 heterostructures tailored via the FGT thickness. Magnetic characterizations and anomalous Hall effect measurements with both out-of-plane and in-plane magnetic fields reveal an enhanced perpendicular magnetic anisotropy (PMA) in thinner FGT and a ferromagnetic order up to room temperature. The pronounced unconventional Hall effect (UHE) suggests the possible formation of skyrmions. The thickness-dependent asymmetric magnetoresistance reveals a unique magnetization switching process. Our results demonstrate the high potential of all-epitaxial FGT/WSe_2 heterostructures for the advancement of future 2D spintronic applications.

DS 3.9 Mon 17:15 H3

Effect of Ni-doping on the structural/magnetic properties of large area epitaxial 2D-ferromganet Fe_3GeTe_2 — •Kacho Imtiyaz Ali Khan[1], Tauqir Shinwari[1], Hua Lv[1], Frans Munnik[2], Jens Herfort[1], Michael Hanke[1], and Joao Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]Helmholtz-Zentrum Dresden- Rossendorf e.V. Dresden, Germany

2D ferromagnets with strong perpendicular magnetic anisotropy exhibit magnetic order down to the monolayer thickness and have the potential to overcome long-term challenges faced by 3D ferromagnets to build up advanced energy-efficient spintronic devices. In this work, we show the large-area epitaxial growth of Ni-doped Fe_3GeTe_2 films via molecular beam epitaxy. X-ray diffraction measurements demonstrate high-quality epitaxy of pure Fe_3GeTe_2 phase on graphene/SiC(0001) substrates. Magneto-transport measurement unveils the ferromagnetic nature of the film, with strong perpendicular magnetic anisotropy for pure Fe_3GeTe_2 and Ni-doped films. However, the Ni-doped Fe_3GeTe_2 shows a decrease in Curie temperature T_C with an increase in Ni-doping. We believe that the Ni doping modifies the lattice parameters and structure (e.g., Ni intercalation), which results in the dilution of magnetic properties of Fe_3GeTe_2 by reducing the T_C down to 50 K. Our findings show the role of Ni incorporation on the ferromagnetic behavior of Fe_3GeTe_2 films, which is crucial for the development of future spintronic devices.

DS 3.10 Mon 17:30 H3

The epitaxial growth of Gallium Selenide — Michele Bissolo, Marco Dembecki, Florian Rauscher, Jan Schabesberger, Abhilash Uhle, Jonathan J. Finley, Gregor Koblmüller, and •Eugenio Zallo — Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München, Garching, Germany

Group III-VI post-transition metal chalcogenides (PTMC, M={In,Ga} and C={S,Se,Te}) are van der Waals semiconductors with layer-dependent electronic, thermoelectric and optical properties, strong photoresponsivity, and a Caldera type valence band [1]. However, the limited scalability and risk of contamination of the standard mechanical exfoliation technique are detrimental to developing devices at an industrial scale. Here, we demonstrate the molecular beam epitaxy growth of PTMC [2] GaSe on 2-inch sapphire wafers. To study the pristine properties of this air-sensitive material in situ, we perform Raman spectroscopy in a UHV chamber directly connected to the growth chamber. Film composition and morphology are investigated by tuning the growth temperature and group VI/III flux ratio and by correlating them with the known spatial gradients across the whole substrate. The combination of these findings with ex-situ surface morphology characterization allows us to construct the phase diagram and identify the 2D layered region [3]. Perspectives on the growth of PTMC on 2D substrates and the epitaxial registry will be discussed. [1] H. Cai, et al., Appl. Phys. Rev. 6, 041312 (2019).[2] E. Zallo, et al., npj 2D Mater. & Appl. 7, 19 (2023).[3] M. Bissolo, et al., [to be submitted].