DS 12: 2D Materials I

Time: Wednesday 9:30–12:00 Location: REC/C213

DS 12.1 Wed 9:30 REC/C213

Purcell enhancement of photocurrent in a van der Waals self-cavity — •Xinyu Li — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

We report the observation of Purcell-enhanced terahertz (THz) photocurrent emission in exfoliated flakes of the van der Waals (vdW) semimetal WTe_2, which act as intrinsic plasmonic self-cavities. Unlike conventional cavities that require external mirrors, micron-scale vdW flakes confine electromagnetic fields via edge reflections, supporting standing-wave plasmonic modes in the THz range. Using ultrafast optoelectronic circuitry, we measured coherent near-field THz emission resulting from nonlinear directional photocurrents excited at crystal edges. Emission spectra reveal resonant enhancement at discrete frequencies, tunable by excitation fluence and device geometry. We attribute this effect to cavity-modified photonic density of states - i.e., the Purcell effect - acting on driven, nonlinear transport currents. An analytical model capturing the self-cavity resonance conditions accurately reproduces experimental trends across multiple devices. Our findings establish WTe_2 as a bias-free, geometry-tunable THz emitter and demonstrate the potential of self-cavity engineering for controlling nonlinear, nonequilibrium dynamics in quantum materials.

Further details are available at arXiv:2507.07987.

DS 12.2 Wed 9:45 REC/C213

Radial Rashba spin-orbit fields in commensurate twisted transition-metal dichalcogenide bilayers — •Thomas Naimer[1], Paulo E. Faria Junior[2], Klaus Zollner[1], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, University of Central Florida, Orlando, Florida 32816, USA

In commensurate twisted homobilayers, purely radial Rashba spin-orbit fields can emerge. We employ first-principles calculations to investigate the band structures and the spin-orbit fields close to the high-symmetry points K and Γ of several commensurate twisted transition-metal dichalcogenide homobilayers: WSe_2, $NbSe_2$, and WTe_2. The observed in-plane spin textures can for the most part be reproduced successfully using a model Hamiltonian, enabling us to extract relevant parameters. Exploring different lateral displacements between the layers, we confirm that the relevant symmetry protecting the radial Rashba is an in-plane 180° rotation axis. Our calculations on WTe_2 bilayers show that their lack of C_3 symmetry results in spin textures that are neither radial nor tangential. All authors acknowledge support by the FLAG ERA JTC 2021 project 2DSOTECH, the European Union Graphene Flagship project 2DSPIN-TECH (grant agreement No. 101135853) and SFB 1277 (Project-ID 314695032).

DS 12.3 Wed 10:00 REC/C213

Spatially Controlled Photoelectrochemical Thinning of 2D Transition Metal Dichalcogenides — •Simon Wörle[1], Lukas Wolz[1], Sergej Levashov[1], Franz Gröbmeyer[2], Johanna Eichhorn[1], Emiliano Cortes[2], Jeremy Robinson[3], and Ian Sharp[1] — [1]Technical University of Munich — [2]Ludwig Maximilian University of Munich — [3]U.S. Naval Research Laboratory

The integration of two-dimensional transition metal dichalcogenides (TMDs) into functional devices and catalytic systems requires detailed understanding and control of their behavior in reactive environments. Here, we systematically investigate the photoelectrochemical (PEC) stabilities of MoS_2, WS_2, $MoSe_2$, and WSe_2 mono- and multilayer flakes under dark and illuminated conditions, revealing two distinct oxidation mechanisms. In the dark, anodic potentials promote oxidation at defect-rich TMD edge sites, with subsequent dissolution of the oxidized species causing progressive lateral shrinkage, while the basal planes remain stable. Under white light illumination from a solar simulator, photoexcited holes drive electrochemical thinning of TMD multilayer flakes, which proceeds at anodic potentials lower than those required for lateral edge oxidation in the dark. This PEC-driven thinning enables controllable top-down fabrication of large-area TMD films with well-defined thicknesses. Importantly, the use of a focused laser beam rather than white light illumination enables precise spatial control over the PEC oxidation process, allowing localized patterning and thinning in predefined regions for the processing and integration of 2D materials into functional devices.

DS 12.4 Wed 10:15 REC/C213

Pairing symmetry of Ising superconductors via the upper critical field — •Lena Engström[1], Ludovica Zullo[2], Tristan Cren[3], Andrej Mesaros[1], and Pascal Simon[1] — [1]Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405 Orsay, France — [2]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [3]Sorbonne Université, CNRS, Institut des Nanosciences de Paris, UMR7588, F-75252 Paris, France

Several conflicting predictions have been made for the symmetry of the pairing in transition metal dichalcogenide (TMD) superconductors. An indication of if singlet or triplet pairing is present can be given by the upper critical field (Hc2), the magnetic field required to fully suppress superconductivity. Monolayer 1H-NbSe2 and 1H-TaS2 have extremely large critical fields, due to a large Ising spin-orbit coupling (SOC), yet they do not scale with SOC and temperature as expected for other TMDs. In our work on few-layer 2H-stacked TMDs, we highlight that the Ising SOC has nodal lines in the Brillouin zone imposed by symmetry. By deriving the susceptibility, we have found that the scaling of the critical field can be traced back to whether the Fermi surface intersects with these lines or not. Reinterpreting existing experimental data, we find that a predominantly singlet order is consistent with the measured Hc2. We propose two experiments where a signature of spin-singlet pairing would be visible, while discussing the possibility of mixed-parity pairing.

DS 12.5 Wed 10:30 REC/C213

Single-Metal-Atom Chains in Transition-Metal Dichalcogenides: Electronic, Magnetic, and Catalytic Properties — •Prosun Santra, Mahdi Ghorbani-Asl, and Arkady V. Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

One-dimensional metallic nanostructures exhibit Peierls instabilities, Tomonaga-Luttinger liquid behavior, Majorana fermions, and half-metallicity, which is interesting in the context of spintronics. Stable single-metal-atom chains (SMACs) were experimentally manufactured by embedding transition metal (TM) atoms at mirror twin boundaries (MTBs) in MoS_2. Using DFT calculations, we study the energetics and properties of SMACs formed by 21 TM elements embedded in MTBs in 2D $MoSe_2$, $MoTe_2$, WS_2, and WSe_2. Spin-polarized calculations reveal localized magnetism and half-metallicity in multiple systems, ideal for nanoscale spintronics. We further study the catalytic properties of these systems. Our results indicate that selected SMACs can surpass Pt(111) in hydrogen evolution reaction activity, so that these defect-engineered structures not only are versatile 1D quantum-spintronic platforms, but may also be utilized as low-cost, high-performance electrocatalysts for green H_2 production.

15 min. break

DS 12.6 Wed 11:00 REC/C213

Magnetoelectric flat band induced by a $\sqrt{3} \times \sqrt{3}$ charge density wave in monolayer $CrSe_2$ — •Victor Pardo[1], Pablo Savino Real[1], Carmen Fuente Santiago[1], Jan Phillips[2], Javier Corral Sertal[1], Adolfo Otero Fumega[3], and Santiago Blanco Canosa[4] — [1]Instituto de Materiais iMATUS, Universidade de Santiago de Compostela, E-15782 Campus Sur s/n, Santiago de Compostela, Spain — [2]Iberian International Nanotechnology Laboratory, INL Braga, Portugal — [3]Department of Applied Physics, Aalto University, 02150 Espoo, Finland — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain

We investigate the electronic and magnetic properties of the $\sqrt{3} \times \sqrt{3}$ charge-density-wave (CDW) phase of $CrSe_2$ using first-principles calculations within density functional theory. We find that the most stable configuration corresponds to a ferromagnetic ground state, which hosts a remarkably flat electronic band exactly at the Fermi level. We show that the flat band derives from an a_{1g}-like component of the Cr t_{2g} manifold in a trigonal environment, combined with bonding–antibonding splittings induced by the formation of Cr trimers in the CDW structure. Strong hybridization between Cr d and Se p orbitals is

crucial for stabilizing this band exactly at the Fermi level. Spin–orbit coupling affects only the remaining *d* bands, leaving the flat band intact. We establish how to tune the existence of this flat-band by relating it to the electric polarization caused by the CDW, hence describing a mechanism to turn on/off strong correlations with an external tuning parameter such as an electric field.

DS 12.7 Wed 11:15 REC/C213

Topological Superconductivity in $NbSe_2$-based Ising-Type Superconductors — •Jozef Haniš[1], Marko Milivojević[2], Zoltan Tajkov[3], and Martin Gmitra[1] — [1]Institute of Experimental Physics SAS Watsonova 47 040 01 Košice, Slovak Republic — [2]Institute of Informatics, Slovak Academy of Sciences, Dúbravská cesta 9 845 07 Bratislava 45, Slovakia — [3]Eötvös Loránd University, Pázmány Péter sétány 1/A, Budapest, Hungary

Topological superconductivity offers the promise of Majorana-bound states for fault-tolerant computation. We develop a symmetry-guided framework for superconducting pairing in Ising-type transition metal dichalcogenides, focusing on $NbSe_2$-based systems. We identify multiple topological phases–classified by Chern numbers and $\mathbb{Z}_2$ invariants–enabled by spin-orbit-induced triplet pairing. We present topological phase diagrams for different doping regimes and discuss zigzag-ribbon band-structure calculations. This work was supported by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I05-03-V02-00071, and the Slovak Academy of Sciences project IMPULZ IM-2021-42.

DS 12.8 Wed 11:30 REC/C213

Modeling Pressure-Induced Exciton Screening in hBN/WSe2/hBN Heterostructures — •Adlen Smiri[1], Shalini Badola[2], Amit Pawbake[2], Clément Faugéras[2], and Iann C. Gerber[1] — [1]Université Fédérale de Toulouse Midi Pyrénées, INSA-CNRS-UPS, LPCNO, 135 Av. de Rangueil, 31077 Toulouse, France — [2]Laboratoire National des Champs Magnétiques Intenses, LNCMI-EMFL, CNRS UPR3228, Univ. Grenoble Alpes, Univ. Toulouse, Univ. Toulouse 3, INSA-T, Grenoble and Toulouse, France.

Hydrostatic pressure is an effective tool to tune excitonic properties in two-dimensional semiconductors. We investigate the pressure dependence of excitonic Rydberg states in a WSe2 monolayer encapsulated in hBN and observe a reduction of the 1s-2s and 1s-3s energy separations with increasing pressure. First-principles calculations indicate negligible changes in the band structure and effective masses, pointing to pressure-modified dielectric screening as the main mechanism. A microscopic dielectric model for the WSe2 monolayer with an effective vacuum gap reproduces the observed excitonic shifts, demonstrating that enhanced screening governs exciton renormalization. These results provide a quantitative framework for tuning excitonic interactions in van der Waals heterostructures.

DS 12.9 Wed 11:45 REC/C213

Above room temperature ferromagnetism in wafer-scale Fe_3GaTe_2/SiC and the origin of double-step hysteresis in MBE-grown Fe_3GaTe_2 films — •Tauqir Shinwari[1], Victor Ukleev[2], Chen Luo[2], Kacho Imtiyaz Ali Khan[1], Florin Radu[2], and Joao Marcelo Jordao Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Helmholtz Zentrum Berlin for Materialien und Energie, Albert-Einstein Straße 15, 12489 Berlin, Germany

Two-dimensional (2D) magnetic materials provide a versatile platform for next-generation spintronic devices, where scalable growth and robust ferromagnetism are the key factors. Fe_3GaTe_2 is a 2D ferromagnet with a high Curie temperature ($\sim$ 360K) and strong perpendicular magnetic anisotropy, making it a particularly promising candidate for energy-efficient spin-based technologies. Until now, most studies on Fe_3GaTe_2 have relied on millimeter-sized bulk crystals and exfoliated flakes, which are unsuitable for wafer-scale integration and reproducible device processing. In this work, we demonstrate high-quality, large-area epitaxial growth of Fe_3GaTe_2 thin films directly on SiC(0001) substrates by MBE. The films exhibit robust above-room-temperature ferromagnetism together with strong out-of-plane magnetic anisotropy, as confirmed by magnetometry and element-specific x-ray techniques. A double-step hysteresis loop is observed in MBE-grown Fe_3GaTe_2 films, pointing to the coexistence or coupling of distinct magnetic subsystems, which will be discussed in the context of Fe site selectivity, thickness dependence, and interfacial effects.