Let's give it a spin!

Wednesday 21 May 2025 - Friday 23 May 2025

Belgrade

Programme

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Wednesday 21 May 2025

Registration - Science Technology Park (08:30 - 09:00)

wednesday morning - Science Technology Park (09:00 - 12:00)

-Conveners: Milivojevic, Marko (Institute of Informatics, Slovak Academy of Sciences)

Lifting spin degeneracy of van der Waals antiferromagnets by polar stacking (09:00, 30 minutes)

Presenter: TSYMBAL, Evgeny

Spin-split antiferromagnets have significance for antiferromagnetic (AFM) spintronics due to their momentum dependent spin polarization which can be exploited for the control and detection of the AFM order parameter. While many 3D antiferromagnets exhibiting non-relativistic spin splitting (NRSS) in their electronic band structure have been proposed and demonstrated, such property remains scarce in 2D systems. Here, we propose polar layer stacking of AFM-ordered van der Waals (vdW) bilayers driving the emergence of NRSS. Based on the spin-space group approach, we identify several representative vdW antiferromagnets which exhibit different types of NRSS when stacked into a polar bilayer. We demonstrate that NRSS can have both altermagnetic and non-altermagnetic origins and elucidate symmetry requirements for NRSS to be switchable by electric polarization. Potentially, the electric polarization switching of NRSS in AFM polar bilayers may be more practical for device applications than spin-orbit torque induced switching of the AFM order parameter.

Non-Relativistic Spin Currents and Torques in Antiferromagnets (09:30, 30 minutes)

Presenter: ZELEZNY, Jakub (Institute of Physics of the Czech Academy of Sciences)

Contrary to the early understanding of antiferromagnets as limited compared to ferromagnets, a rich landscape of phenomena in antiferromagnets has been demonstrated that could be utilized for various spintronics functionalities. Here, we discuss recent advances in understanding of how electrical current can induce spin currents or spin torques in antiferromagnetic systems, focusing primarily on non-collinear antiferromagnets and on phenomena that originate from the non-collinear order without requiring the relativistic spin-orbit coupling. We show that antiferromagnets can host spin-polarized currents and that these can be utilized for magnetic junctions, that antiferromagnets can be used for spin-charge conversion, potentially even without any spin loss, and that a non-relativistic current-induced torque analogous to the spin-orbit torque can exist in antiferromagnets.

Non-collinear magnetism in 2D materials from first principles: Magnetoelectricity and type II multiferroic order (10:30, 30 minutes)

Presenter: OLSEN, Thomas (Technical University of Denmark)

We present a systematic classification of the magnetic ground states in hundreds of two-dimensional (2D) materials. Non-collinear order is shown to be abundant and may typically be represented by planar spin spiral ground states. We discuss a range of physical effects associated with non-collinear order and take specific materials as examples. The Ni(Cl,Br,I)$_2$ compounds exhibit type II multiferroic order where the spontaneous polarization is induced by spiral order and we discuss the subtleties associated with the calculation of the polarization from first principles. The breathing Kagomé compounds Nb$_3$(Cl,Br,I)$_8$ are pyroelectric and have spiral ground states with ordering vectors that couple strongly to out-of-plane external electric fields. Finally we discuss a set of 2D altermagnets and analyse the important role of spin-orbit coupling with respect to the band structure, magnons and non-collinearity.

Magnetoelectricity of Topological Solitons in 2D Magnets (11:00, 30 minutes)

Presenter: BARONE, Paolo (Institute Superconductors, Innovative Materials and Devices, Consiglio Nazionale delle Richerche (CNR-SPIN))

Magnetoelectricity, accounting for the coupling between electric and magnetic dipoles, has attracted a revived interest in the last few decades. The interest was largely fueled by the renaissance of multiferroicity where coexisting electrical and magnetic degrees of freedom may couple, as indeed happens in type-II multiferroics displaying an electric polarization induced by a symmetry-breaking modulation of the magnetization. Spatially localized magnetic structures such as domain walls or Skyrmions may also sustain a net electric dipole moment ultimately arising from magnetoelectric coupling, in principle enabling their control via electric field. In this respect, magnetoelectric effects can play an important role in two-dimensional magnets, where a moderate voltage is sufficient to produce a huge electric field perpendicular to the 2D magnet layer. Despite being spatially localized, topological magnetic solitons typically extend over length scales of at least several nanometers, leaving them beyond reach of direct ab initio calculations. To solve this critical issue, we developed a multiscale approach to magnetoelectricity that bridges atomistic and continuum models, with all parameters fully determined from first principles. We carefully validate and apply our approach to the prototypical 2D ferromagnet CrI$_3$, studying the electric polarization of different realizations of spin spirals as well as of magnetic topological solitons in the form of domain walls and Skyrmions or anti-Skyrmions. After providing general symmetry requirements for the magnetoelectric coupling tensor in both atomistic and continuum model, we formally show that the magnetoelectric parameters of our models are equivalent to electric-field induced Dzyaloshinskii-Moriya interactions, further

allowing us to address electric-field stabilization of non-collinear spin structures.

Orbital magnetization from charge current parallel to an interface: a non-Hall effect mechanism (11:30, 15 minutes)

Presenter: TITOV, Mikhail (Radboud University, Nijmegen, the Netherlands)

Magnetization in solids arises from both orbital and spin degrees of freedom. While spin-related effects, such as the spin Hall and inverse spin Hall effects, have been widely considered the dominant mechanisms in magnetoelectric phenomena, recent experimental evidence suggests a much more significant role for orbital contributions than previously expected. This has led to the development of the concept of the orbital Hall effect. Here, we present an alternative perspective on orbital physics in metals and semiconductors subjected to charge currents. It is well established that a non-equilibrium orbital magnetic moment can emerge in conductors due to skew scattering from asymmetric impurities. We highlight that a similar skew-scattering mechanism can also be induced by conductor boundaries, even in the absence of special impurities. Specifically, we propose that a high-quality, flat interface can act as a long-range skew scatterer for charged quasiparticles. When an electric current flows parallel to the interface, an imbalance in clockwise and counterclockwise scattering leads to a net orbital magnetization. This magnetization is strongest at the interface and decays linearly in the perpendicular direction. We suggest that this effect can be experimentally detected through spatially resolved Kerr effect measurements at distances up to the electron phase coherence length from the interface. Unlike the orbital Hall and orbital Edelstein effects, this phenomenon does not rely on bulk inversion symmetry breaking and is fundamentally distinct from Hall physics.

Boosting spin-orbit torque through intra-particle entanglement in Dirac materials. (11:45, 15 minutes)

Presenter: MEDINA DUEÑAS, Joaquín (ICN2)

The spin-orbit torque (SOT) mechanism offers new avenues for magnetic technologies, where spin-orbit coupling (SOC) at a metal-magnet interface is harnessed to electrically manipulate the magnetic state. Van der Waals materials emerge as a natural SOT platform due to their layered structure, where furthermore SOC and magnetic properties can be tailored by proximity effects. However, low SOT efficiencies and the need for experimentally challenging low-symmetry materials still hinder their progress, requiring new developments to further boost the efficiency and control of SOT mechanisms. In this work we unveil novel SOT and charge-to-spin conversion mechanisms due to intra-particle entanglement between spin and pseudospin in graphene-based heterostructures [1, 2]. We begin demonstrating the manipulation of spin-pseudospin entanglement by tuning different forms of proximity-induced SOC. By these means we achieve charge-to-spin conversion of maximal efficiency in non-magnetic graphene via the Rashba-Edelstein effect (also called inverse spin galvanic effect). Upon proximitizing a magnetic layer, additional SOT mechanisms originated within the Fermi sea are enabled. Using a semi-classical theory for the non-equilibrium spin dynamics we trace the breakdown of the semi-classical behavior due to predominance of quantum spin-pseudospin entanglement, leading to an enhanced SOT regime. Here, we unveil a novel SOT contribution which emerges within the topological gap of the quantum anomalous Hall phase. Overall, our results reveal that intertwined spin-pseudospin mechanisms lead to novel SOT phenomena which may serve to further tailor spintronic technologies. ### References [1] **J. Medina Dueñas**, J.H. Garcia and S. Roche, *Phys. Rev. Lett.* **132**, 266301 (2024) [2] **J. Medina Dueñas**, J.H. Garcia and S. Roche, arXiv:2408.16359 (2024)

time	title	presenter
10:00	Coffee break (30 minutes)	

Lunch break - Science Technology Park (12:00 - 13:45)

wednesday afternoon - Science Technology Park (13:45 - 17:05)

-Conveners: Martin Gmitra

Spin proximity effects in 2D van der Waals heterostructures (13:45, 30 minutes)

Presenter: FABIAN, Jaroslav (University of Regensburg)

The emergence of 2D materials has transformed solid-state physics. The key factor driving research into 2D materials is the ability to efficiently control the atomic-scale physical properties of monolayers and their heterostructures, which involve weak yet important van der Waals interactions. Spintronics aims to utilize the spin of conduction electrons to develop devices like spin transistors and tunneling junctions. Since the early experiments in graphene, spintronics has advanced, establishing a solid understanding of spin physics in monolayers. Current research focuses on van der Waals heterostructures, which serve as tailored platforms to explore new spintronic phenomena. Tuning electron spin properties in these structures mainly relies on the proximity effect. For instance, ferromagnetic graphene can be created by stacking it with 2D ferromagnetic semiconductors. Additionally, such spin properties of graphene's itinerant electrons can be tuned through methods like gating and twisting. By combining ferromagnets with strong spin-orbit materials, unique structures can be created that allow for tunable spin interactions. In this talk, I will discuss the recent advances in spin proximity phenomena, but also potential applications related to spin-charge

conversion and spin-orbit torques. Funding from CRC1277, EU 2DSPIN-TECH, and SPP2244 is acknowledged.

Density matrix and dissipation in spin transport and dynamics: Applications to spin-orbit torque and exciton-mediated optical excitation of magnons (14:15, 30 minutes)

Presenter: NIKOLIC, Branislav (University of Delaware)

The density matrix is a fundamental quantity of nonequilibrium quantum statistical mechanics, introduced in 1927 shortly after the birth of quantum physics by von Neumann and Landau, which allows us to compute observable quantities in spintronics like spin torque, spin densities, spin currents etc. However, debates have been raging in recent spintronic literature on how to construct density matrix properly in linear-response stead-state nonequilibrium via Kubo or Keldysh formulas, as their recent usage has produced apparently vastly different physical conclusions. For time-dependent systems, such as 2D antiferromagnet CrSBr driven by femtosecond laser pulses, one further needs to properly construct a time-dependent density matrix and include excitons within it to explain very recent experiments on optical excitation of magnons via exciton mediation. This talk will explain recently achieved full resolution [1] of “debates raging in the literature” via examples of spin-orbit torque [2] in proximitized graphene, computed via both Kubo and Keldysh formulas for the density matrix with proper inclusion of dissipation effects; as well as explain [3] how magnons, of finite life-time due to dissipation, are optically excited in CrSBr and how they can be detected via new signatures in pumped current or emitted electromagnetic radiation. [1] S. M. João, M. D. Petrović, J. M. Viana Parente Lopes, A. Ferreira, and B. K. Nikolić, arXiv:2408.16611 (2024). [2] K. Dolui, M. D. Petrović, K. Zollner, P. Plecháč, J. Fabian, and B. K. Nikolić, Nano Lett. **20**, 2288 (2020). [3] J. Varela-Manjarres, Y. Ren, and B. K. Nikolić, in preparation.

Magnetism and spin transport in 2D magnet based van der Waals heterostructures (15:15, 30 minutes)

Presenter: SANYAL, Biplab (Uppsala University, Sweden)

In recent years, the realization of magnetic long-range order in atomically thin 2D materials has shown a big potential in spintronic applications in ultrathin magnets due to the possibility of manipulation of magnetism by external fields, strain or proximity effects in van der Waals (vdW) heterostructures. Specifically, the family of 2D metallic magnets Fe$_n$GeTe$_2$ ($n=3, 4, 5$) has attracted a huge attention due to their high Curie temperatures and intriguing properties. A systematic study of the electronic structure and magnetism of Fe$_n$GeTe$_2$ magnets by ab initio density functional theory, calculations of interatomic exchange interaction parameters and Monte Carlo simulations will be shown highlighting the importance of electron correlation with the aid of dynamical mean field theory, spin-orbit coupling and effects of transition metal doping. Also, results on spin-polarized quantum transport calculations will be presented for PtTe$_2$/Fe$_4$GeTe$_2$/PtTe$_2$ van der Waals heterostructures. Finally, the effects of electrode polytypes on spin transport properties will be shown for a vdW heterostructure comprising of a ferromagnetic monolayer of 1T-VSe$_2$ with two structural polytypes (1T and 2H) of TaS$_2$ electrodes. It will be shown that the 1T-device shows superior performance with lower Gilbert damping, reduced critical current density and voltage for magnetization switching, compared to the 2H-device, which requires significantly higher current and voltage. [1] S. Ghosh, S. Ershadrad, V. Borisov, B. Sanyal, npj comp. mat. 9, 86 (2023). [2] S. Ershadrad, S. Ghosh, D. Wang, Y. Kvashnin, B. Sanyal, J. Phys. Chem. Lett. 13, 4877 (2022). [3] S. Ghosh, S. Ershadrad, B. Sanyal, 2D materials 11, 035002 (2024). [4] M. Davoudiniya, B. Sanyal, Nanoscale Adv. 6, 6278 (2024). [5] R. Ngaloy et al., ACS Nano 18, 5240 (2024). [6] M. Davoudiniya, B. Sanyal, npj 2D Mater. Appl. (in press)

The spin accumulation in graphene on 1T-TaS$_2$ using the linear response theory. The effect of a perpendicular electric field. (15:45, 15 minutes)

Presenter: MNICH, Juraj (Pavol Jozef Šafárik University in Košice, Faculty of Science, Institute of Physics)

In the last decades, proximity effects in graphene-based van der Waals heterostructures have acquired significant attention for their high tunability [1]. Here we study current induced spin accumulation in graphene proximitized by monolayer of 1T-TaS$_{2}$. In such heterostructure, the proximity-induced spin-orbit coupling in the graphene is directly related to the correlated electronic states due to the emergence of charge density wave in 1T-TaS$_{2}$ [2] at low temperatures [3]. The current-induced spin accumulation in the proximitized graphene is directly related to the charge to spin conversion efficiency. The spin accumulation has been calculated in linear Kubo response regime as a function of chemical potential for different perpendicularly applied electric fields. The effective Hamiltonian considers low energy π bands and proximity induced intrinsic and Rashba spin-orbit coupling terms. We studied charge to spin conversion efficiency for different graphene/1T-TaS$_2$ and 1T-TaS$_2$/graphene/1T-TaS$_2$ stacking configurations and investigated the effect of the perpendicular electric field on conventional and unconventional Rashba-Edelstein effect. We found that for the specific stacking preserving the horizontal mirror plane symmetry, the perpendicular electric field can be used as an effective control knob to switch sign of the spin accumulation. ### Acknowledgements This work has been funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V05-00008. ### References [1] M. Gmitra and J. Fabian, “Proximity Effects in Bilayer Graphene on Monolayer WSe$_2$: Field-Effect Spin Valley Locking, Spin-Orbit Valve, and Spin Transistor,” Physical Review Letters, vol. 119, no. 14. American Physical Society (APS), Oct. 04, 2017. doi: 10.1103/physrevlett.119.146401. [2] K. Szałowski, M. Milivojević, D. Kochan, and M. Gmitra, “Spin–orbit and exchange proximity couplings in graphene/1T-TaS$_2$ heterostructure triggered by a charge density wave,” 2D Materials, vol. 10, no. 2. IOP Publishing, p. 025013, Feb. 23, 2023. doi: 10.1088/2053-1583/acbb19. [3] D. C. Miller, S. D. Mahanti, and P. M. Duxbury, “Charge density wave states in tantalum

dichalcogenides," Physical Review B, vol. 97, no. 4. American Physical Society (APS), Jan. 17, 2018. doi: 10.1103/physrevb.97.045133.

Proximity-Induced Self-Torque in Graphene/1T-TaS$_2$ (16:00, 15 minutes)

Presenter: RASSEKH, Maedeh (Institute of Physics, Pavol Jozef Šafárik University in Košice)

Spin-orbit torque (SOT) in van der Waals heterostructures offers a pathway to energy-efficient spintronic devices. The proximity of a transition-metal dichalcogenide to graphene can have a profound effect on the induced magnetism and spin texture of graphene. One of the promising materials for SOT research is 1T-TaS$_2$. A monolayer of 1T-TaS$_2$ comprises strong spin-orbit coupling, charge density wave correlated phase with a David star pattern, and spontaneous in-plane magnetization. When a layer of graphene is placed on 1T-TaS$_2$ monolayer, a spin-orbit coupling and exchange interaction is proximitized to the graphene electronic structure. This enables the generation of self-induced torque on graphene electrons when a charge current passes through the graphene. Using a tight-binding model with parameters fitted to density functional theory data, combined with quantum transport simulations, we compute spin-orbit torques for a range of Fermi levels to simulate electron and hole doping. We quantify the contributions to the self-torque originating from exchange interaction, intrinsic spin-orbit coupling, and Rashba spin-orbit coupling. Our results reveal that the stacking configuration of graphene on 1T-TaS$_2$ plays a critical role in the strength of the spin-orbit torque. Specifically, when graphene is aligned in a top stacking configuration where a carbon atom is placed over the Ta atom of the David star center, the torque values are significantly larger, by nearly an order of magnitude, compared to the hollow case where the center of the graphene ring and the David star are placed on top of each other. These findings not only deepen our understanding of SOT mechanisms in graphene/1T-TaS$_2$ heterostructures but also offer valuable insights for the design and optimization of spintronic devices based on such systems. ### Acknowledgements Funded by the European Union's NextGenerationEU program through the Recovery and Resilience Plan for Slovakia under the Project No. 09I03-03-V04-00318.

Radial Rashba spin-orbit fields in commensurate twisted transition-metal dichalcogenide bilayers (16:15, 15 minutes)

Presenter: Dr NAIMER, Thomas (University of Regensburg)

In commensurate twisted homobilayers, purely radial Rashba spin-orbit fields can emerge due to the interaction of the twisted hidden Rashba spin-orbit coupling (SOC) from each layer [1]. We calculate the band structures and the spin-orbit fields close to the high symmetry points K and Γ of commensurate twisted transition-metal dichalcogenide homobilayers (WSe$_2$ and NbSe$_2$) from first principles using density functional theory (DFT) calculations. The observed in-plane DFT spin textures are mostly radial and can in large parts be described by a model Hamiltonian, which consists of two continuum models for the two layers, including SOC terms and interacting by a general (spin-conserving) interlayer coupling. We additionally investigate the effects of an electric field, different lateral shifts and increasing interlayer distance, all three of which can bring back the radial Rashba structure to a tangential one. ### Acknowledgements We acknowledge support by the FLAG ERA JTC 2021 project 2DSOTECH. T.N. and J.F. were also supported by the European Union Horizon 2020 Research and Innovation Program 881603 (Graphene Flagship). ### References [1] Frank et al, "Emergence of radial Rashba spin-orbit fields in twisted van der Waals heterostructures", Physical Review B **109**, L241403 (2024).

Spin model of graphene triangulenes embedded in hexagonal boron nitride (16:30, 15 minutes)

Presenter: TIBOR POZSÁR, Dániel (Eötvös Loránd University, TRILMAX)

We are investigating triangulene shaped substitutional defects in hexagonal boron nitride filled with carbon atoms. We show how the triangulene shaped defects encompass magnetic moments and with ab initio methods we build Heisenberg like classical spin models representing their interactions. We show how different lattice terminations and sizes impact the magnetic properties of the system.

time	title	presenter
14:45	Coffee break (30 minutes)	

Thursday 22 May 2025

thursday morning - Science Technology Park (09:00 - 12:00)

-Conveners: Šljivančanin, Željko (Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade)

Dissipative and nondissipative dynamics excited by spin torques in a quantum dot (09:00, 30 minutes)

Presenter: GAMBARDELLA, Pietro (ETH Zurich)

Spin torques are central to spintronics, enabling current-induced magnetization switching, domain wall motion, and resonant magnetic oscillations in nanoscale devices. While most studies describe spin torques in semi-classical terms, probing their action at the level of a single spin reveals their fundamentally quantum nature. Electron paramagnetic resonance (EPR) performed via scanning tunneling microscopy (STM) offers coherent control over individual spins along with direct insight into their interaction with electric currents and the surrounding environment. In this talk, I will show that EPR of a single spin in a pentacene molecule can be driven by a time-dependent spin-polarized current injected from the STM tip. Depending on the tunnelling regime, the molecular spin exhibits either coherent or incoherent dynamics, whereby spin rotations and decoherence are controlled by the applied voltage and current. These results offer a unique perspective on how electric currents influence quantum spin states, in contrast with the established action of time-dependent electromagnetic fields. Spin torques also enable to excite EPR in regimes where the thermal spin polarization is too low to yield an observable EPR signal by an oscillating magnetic field.

Spin and Orbital Currents in Two-Dimensional Layered Materials (09:30, 30 minutes)

Presenter: Prof. FERREIRA, Aires (University of York)

Abstract body goes here.Spin-orbit coupling (SOC)—a relativistic interaction which entangles a particle's motion with its quantum mechanical spin—is fundamental to a wide range of physical phenomena, spanning from the formation of topological insulators to the spin Hall effect of light. Recent years have seen remarkable progress in the probing, enhancing and tailoring of SOC in artificial materials, specifically heterostructures, made of two or more individual flakes of graphene-like crystals arranged in a stack. From the electrical control of spin-valley coupling in bilayer graphene to the reversible spin-charge conversion in graphene with proximity-induced SOC courtesy of atomically-thin semiconductors, these discoveries challenge our previous notions on the possible behavior of spin-orbit coupled electrons at hetero-interfaces. In this talk, I will focus on the spin-orbit physics of graphene-based van der Waals heterostructures and show that they are sensitive to the atomic registry between graphene and its high-SOC partner material. This opens up interesting possibilities for spin-charge interconversion, such as a spin Hall effect tunable by means of a simple interlayer rotation angle. A new proposal for the lateral patterning of spin-orbit fields in these systems, leading to pronounced quantum geometric effects, will be briefly discussed. Finally, I will present recent work using accurate transport methods to understand the microscopic origin of orbital Hall effects in realistic (disordered) 2D materials, including the discoveries of an orbital version of skew scattering without SOC and the crucial role played by the symmetries of scattering centers.

Spin and orbital induced dynamics in 2D Magnets (10:30, 30 minutes)

Presenter: DASH, Saroj (Quantum Device Physics Laboratory, Chalmers University of Technology, Gothenburg, Sweden)

Exploring spin, orbital and topological properties of two-dimensional (2D) materials represents a new platform for realizing novel quantum and spin-based phenomena and device applications. Furthermore, engineering 2D heterostructures by combining the best of different materials in one ultimate unit can offer a plethora of opportunities in spintronics. Furthermore, nontrivial topology in the electronic band structure of quantum materials also makes them potential candidates for emerging technologies. We showed that their unique band structure and lower crystal symmetries can provide an unconventional spin polarized current [1] and out-of-plane spin-orbit torque [2] needed for field-free magnetization switching. The out-of-plane spin Hall conductivity in such 2D quantum materials are estimated to be an order of magnitude higher than the conventional materials. 2D magnets are promising due to their tunable magnetic properties, which can be altered through gating and doping, allowing the strength of magnetic interactions to be tailored for specific applications. We reported above room temperature van der Waals magnet-based spin-valve [3,4] and spin-orbit torque memory [5] devices using all-2D heterostructures. In the latter cases, using a TaIrTe$_4$/Fe$_3$GaTe$_2$ device, we could demonstrate energy-efficient and field-free magnetization switching [5]. Furthermore, we utilized van der Waals magnets with the coexistence of ferromagnetic and antiferromagnetic orders, exhibiting intrinsic exchange bias in the system, which gives rise to canted magnetism [6]. Such canted magnetism facilitates field-free magnetization switching in conventional spin-orbit materials, such as Pt [6,7]. Furthermore, I will present some new findings on orbital torque-induced magnetization switching of van der Waals magnets. These findings open a new platform for realizing devices that utilize van der Waals magnets and all-2D heterostructures. ###References: [1] Advanced Materials 32, 2000818 (2020). [2] Nature Communications 15 (1), 4649 (2024). [3]Advanced Materials, 2209113 (2023). [4] ACS Nano 2024, 18, 7, 5240 (2024). [5] Arxiv,https://doi.org/10.48550/arXiv.2308.13408 [6] Arxiv,https://doi.org/10.48550/arXiv.2408.13095 [7] ACS Nano 19, 14, 13817–13824 (2025).

Switchable p-wave magnetism (11:00, 30 minutes)

Presenter: COMIN, Riccardo

Altermagnets are a new class of magnetic materials that combine aspects of ferromagnets and antiferromagnets, possessing zero net magnetization like antiferromagnets but exhibiting (potentially large) spin splitting of the electronic bands and anomalous Hall responses like ferromagnets. Recent research has focused on magnetic systems with odd-parity spin splitting of nonrelativistic origin (p-wave magnets), which are promising for spintronic applications. Symmetry considerations suggest the possibility of coupling altermagnetism with ferroelectricity in polar chiral magnets, potentially allowing for novel mechanisms for electric-field control of magnetism. Nickel iodide (NiI$_2$) is a van der Waals magnetic insulator and multiferroic when in its chiral magnetic phase (T < 59 K). The spin helices (pitch ~ 7 unit cells) that characterize this phase breaks inversion symmetry, leading to an induced electrical polarization of purely electronic origin. I will start by discussing prior work on the evolution of the multiferroic down to the two-dimensional (single-layer) limit. I will then focus on more recent work characterizing the nonrelativistic spin splitting of electronic bands in NiI2, and its connection to symmetry and chirality. I will present a demonstration of the electrical (voltage-based) switching of chirality and consequent reversal of the momentum-space spin polarization. I will conclude with an outlook for potential applications of spin-chiral multiferroics for information storage.

Tuning magnetic exchange interactions in two-dimensional magnets (11:30, 15 minutes)

Presenter: Prof. SZUNYOGH, László (Budapest University of Technology and Economics)

A computational study is presented with the aim to mimic different experimental approaches to tune the magnetic interactions in two-dimensional van der Waals magnets. The tensorial exchange interactions [1] among all relevant atomic pairs are evaluated for CrGeSe$_3$, CrGeTe$_3$, and Janus Cr$_2$Ge$_2$(Se,Te)$_3$ monolayers and their dependence is analyzed on different external parameters, such as biaxial and uniaxial strain, as well as gate voltage. Particular attention is paid to interactions that emerge or vanish due to changes in the system’s symmetry, especially under uniaxial strain and gate voltage. It is found that biaxial and uniaxial strains significantly modify the isotropic exchange couplings, which can lead to a transition from a ferromagnetic to an antiferromagnetic phase, while a gate voltage induces Dzyaloshinskii–Moriya interactions, forming a vortex pattern whose chirality is determined by the sign of the electric field. The electric dipole moment of the Janus material turns out to be large, raising the possibility of multiferroic behavior [2]. ###References [1] Gabriel Martínez-Carracedo, László Oroszlány, Amador García-Fuente, Bendegúz Nyári, László Udvardi, László Szunyogh, and Jaime Ferrer, Phys. Rev. B **108**, 114418 (2023) [2] Gabriel Martínez-Carracedo, Amador García-Fuente, László Oroszlány, László Szunyogh, Jaime Ferrer, Phys. Rev. B **110**, 184406 (2024)

Beyond the orbitally-resolved magnetic exchange (11:45, 15 minutes)

Presenter: ŠABANI, Denis (University of Antwerp)

Magnetic two-dimensional (2D) materials are at the forefront of research in recent years, owing to their rich yet tunable properties, conveniently integrable in spintronic, magneto-electric and multiferroic functional heterostructures and prospective devices. The exploration and manipulation of those properties requires understanding of the microscopic origin of magnetic exchange, which is a pertinent challenge beyond the existing theories. Magnetic 2D materials are typically based on the magnetic exchange between transition-metal (TM) atoms, fostered by the ligand atoms (X). Existing literature offers description of magnetic exchange on atomic level, with occasional attempts to quantify different orbital contributions to the total magnetic exchange between two TM atoms. Moreover, it is known that magnetic exchange between two d orbitals on two TM atoms is in general mediated by p orbital(s) of the X atom(s). However, the exact underlying microscopic mechanisms and the strength of their influence on the magnetic exchange between two d orbitals remain beyond reach. This motivated us to go beyond, and develop a systematic method to quantify all possible mechanisms that contribute to magnetic exchange for an arbitrary pair of atoms in a given material. The foundation of the method lies in the decomposition of the Green's function into different terms, which are explicitly dependent on the matrix elements of first-principles Hamiltonian in a localized basis. We applied it to the archetypal magnetic 2D monolayers, CrI$_{3}$ and NiI$_{2}$, to (1) confirm some of the earlier proposed contributions to the atomic exchange, (2) to reveal previously underrated ones, and (3) to exactly quantify microscopic mechanisms behind both. The work is currently being under revision for publication in Physical Review Letters, and non-peer-reviewed version is available online (see Ref. [1]). ### Acknowledgements This work was supported by the Research Foundation-Flanders (FWO-Vlaanderen). The computational resources and services for this work were provided by the VSC (Flemish Supercomputer Center), funded by the FWO and the Flemish Government - department EWI. ### References [1] D. Šabani et al., Beyond the orbitally-resolved magnetic exchange in CrI$_{3}$ and NiI$_{2}$, https://arxiv.org/abs/2502.08273, (2025).

time	title	presenter
10:00	Coffee break (30 minutes)	

Lunch break - Science Technology Park (12:00 - 13:45)

thursday afternoon - Science Technology Park (13:45 - 17:30)

-Conveners: Droghetti, Andrea (Dipartimento di Scienze Molecolari e dei Sistemi Nanoscopici - Università Ca' Foscari, Venice, Italy)

X-ray magnetic circular dichroism in MnTe and rutile altermagnets (13:45, 30 minutes)

Presenter: KUNES, Jan (Masaryk University, Brno)

X-ray magnetic circular dichroism (XMCD) is a well-established technique for investigating magnetism. Here, we present theoretical studies of XMCD at the manganese L$_{2,3}$ edge in two altermagnets, MnTe [1] and MnF$_2$ [2], with experimental data available for MnTe. Our calculations reveal that spin-orbit coupling in the valence states has a negligible effect on the XMCD spectra. In other words, the spectra computed in an idealized non-relativistic system—where altermagnetism is well-defined by symmetry—closely resemble those obtained in a more realistic model that includes valence spin-orbit coupling. This feature distinguishes XMCD from optical or transport measurements, where spin-orbit coupling is essential for observing magneto-optical or anomalous Hall effects. Using MnTe and MnF$_2$ as examples, we demonstrate that crystal symmetry dictates the origin of the finite XMCD signal, with different terms in the Hamiltonian contributing depending on symmetry. In the case of rutile MnF$_2$, the core-valence exchange interaction causes a minor modification of the XMCD signal, which exists even without this interaction. Conversely, in hexagonal MnTe, the core-valence interaction is necessary to observe any finite XMCD signal at all. These distinct origins of XMCD account for the different magnitudes of the effect in these isolectronic materials (Mn d^5). Finally, we will discuss how XMCD can be utilized to determine the orientation of the Néel vector. ### References [1] A. Hariki et al., Phys. Rev. Lett. 132, 17670 (2024). [2] A. Hariki et al., Phys. Rev. B 110, L100402 (2024).

Electric field control of spin (and valley) polarization in two-dimensional antiferromagnets (14:15, 30 minutes)

Presenter: GIBERTINI, Marco

Antiferromagnetic conductors with suitably broken spatial symmetries host spin-polarized bands even in the absence of spin-orbit coupling, leading to transport phenomena commonly observed in metallic ferromagnets. Here we show that, in the two-dimensional (2D) limit, an electric field can control the relevant symmetries. Two situations are discussed. First, we show by first-principles simulations and magnetotransport experiments that a perpendicular electric displacement field can switch the spin polarization of the conduction band on and off in an antiferromagnetic van der Waals bilayer, such as CrPS$_4$. Second, we consider the case of altermagnets, where spin-valley locking can give rise to band extrema (valleys) at different locations in the Brillouin zone for opposite spins. By screening high-throughput databases of 2D magnetic materials, we find a potential candidate with suitable symmetries, where an electric field can lift the degeneracy between valleys with opposite spin and thus create a simultaneous spin and valley polarization. First-principles simulations predict a sizeable effect that meets the requirements for applications in spin-valleytronics. ### Acknowledgements We acknowledge financial support from Ministero Italiano dell'Università e della Ricerca through the PRIN2022 project SECSY (CUP E53D23001700006), funded by the European Union – NextGenerationEU.

Controlling magnetism in 2D van der Waals materials from first principles (15:15, 30 minutes)

Presenter: BALDOVI, Jose J. (Instituto de Ciencia Molecular (ICMol), University of Valencia)

The recent isolation of two-dimensional (2D) magnets offers tantalizing opportunities for spintronics, magnonics and quantum technologies at the limit of miniaturization. [1] In this presentation, I will provide an overview of our recent results on this fascinating topic. First, we will take advantage of the outstanding deformation capacity of 2D materials to answer the question: Can we use strain engineering to control spin waves propagation? [2] For that, we will focus on the magnetic properties, magnon dispersion and spin dynamics of the air-stable 2D magnetic semiconductor CrSBr, investigating their evolution under mechanical strain and Coulomb screening using first-principles. Then, we will introduce the modulation of the properties of this 2D magnet after the deposition of molecular materials in a journey towards molecular controlled magnonics. [3–5] On the other hand, we will investigate magnetostriction effects in 2D van der Waals antiferromagnets such as FePS$_3$ and CoPS$_3$, [6] create new Janus 2D magnetic materials based in MPS$_3$ in order to answer: what are the effects of mirror broken symmetry on the magnetic properties? [7], and finally, we will delve into the origin of above-room-temperature magnetism in Fe$_3$GaTe$_2$. [8]

Building unconventional magnetic phases on graphene by H atom manipulation: From altermagnets to Lieb ferrimagnets (15:45, 15 minutes)

Presenter: CHOURASIA, Simran (Universidad Autónoma de Madrid)

Engineering all magnetic phases within a single material platform would mark a significant milestone in materials science, simplifying device fabrication by eliminating the need for integrating different materials. We demonstrate that graphene can host all non-relativistic magnetic phases—diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism, ferrimagnetism, altermagnetism and fully compensated ferrimagnetism —using single H atoms as building blocks. Their magnetic character is confirmed by density functional theory and mean-field Hubbard calculations. Notably, altermagnetism can be realized, exhibiting directionally spin-split bands coexisting with zero net magnetization due to spatial symmetries. Furthermore, fully compensated ferrimagnets can be created, lacking these symmetries and presenting unrestricted spin-splitting, with vanishing net magnetization protected by Lieb's theorem. We take this idea to the laboratory and, through precise manipulation of H atoms by scanning tunneling microscopy, experimentally create unit cells of all magnetic phases. These findings open the door to the bottom-up

design of magnetic phases via symmetry selection. We are currently extending our study with transport calculations on these systems, especially to check the polarization in Lieb compensated ferrimagnets and direction dependent polarization in altermagnets. We are also investigating spin-flip excitons on the antiferromagnets obtained from centrosymmetric arrangement of H atoms on graphene with our group's code XATU, aiming to capture some of its magnonic properties. ###References [1] B. Viña-Bausá, M. A. García-Blázquez, S. Chourasia, R. Carrasco, D. Expósito, I. Brihuega, and J. J. Palacios, Building Unconventional Magnetic Phases on Graphene by H Atom Manipulation: From Altermagnets to Lieb Ferrimagnets, arXiv:2501.12329. [2] A. J. Uría-Álvarez, J. J. Esteve-Paredes, M. A. García-Blázquez, and J. J. Palacios, Efficient computation of optical excitations in two-dimensional materials with the Xatu code, Computer Physics Communications 295, 109001 (2024).

Hund interaction induced superconductivity in proximitized Bernal bilayer graphene (16:00, 15 minutes)

Presenter: ZHUMAGULOV, Yaroslav (EPFL)

The impact of proximity-induced spin-orbit coupling and Hund interactions on the correlated phase diagram of Bernal bilayer graphene (BBG) is theoretically investigated. Using an effective ab initio-fitted BBG/WS$_2$ van der Waals heterostructure model, Coulomb and Hund interactions are incorporated through the random-phase approximation to examine possible correlated phases across various displacement fields, doping levels, and temperatures. Findings indicate that Hund interaction and intervalley and Stoner fluctuations can induce superconductivity in proximitized BBG. Spin-orbit coupling, in turn, removes the degeneracy of the superconducting state in the spin subspace, causing a splitting into triplet and singlet states.

Borophenes: Tuning Superconducting Properties via Hydrogenation and Intercalation, and Stabilizing 2D Magnetic Nanostructures (16:15, 15 minutes)

Presenter: ŠOŠKIĆ, Božidar N. (Faculty of Natural Sciences and Mathematics, University of Montenegro & Department of Physics & NANOlab Center of Excellence, University of Antwerp)

Borophene, a two-dimensional (2D) allotrope of boron, exhibits exceptional physical and chemical properties, positioning it as a promising candidate for various practical applications, potentially surpassing graphene [1]. However, its high reactivity and susceptibility to oxidation under ambient conditions present significant challenges. Strategies such as hydrogenation of monolayer [3] and fabrication of bilayer configurations [4] have been proposed to address these issues. Through density functional perturbation theory (DFPT) and anisotropic Migdal-Eliashberg equations, we have identified these configurations as promising superconducting candidates, with hydrogenated β_{12} monolayer achieving superconducting critical temperature (T_C) of approximately 29 K [5], and alkaline-earth metal-intercalated bilayers reaching T_C up to 58 K [6]. These findings further elucidate the absence of superconductivity in bare monolayer borophene, aligning well with experimental observations, and highlighting the role of hydrogenation and intercalation in enhancing and tuning its superconducting properties. Furthermore, by using the spin-dependent density functional theory (SDFT) and the anisotropic Heisenberg model, we explored β_{12} borophene as an ideal platform for stabilization of iron-based 2D magnets, revealing long-range magnetic order due to direct d-orbital interactions and superexchange mechanisms [7]. To overcome oxidation challenges, manganese-intercalated bilayer β_{12} borophene emerges as a robust solution, maintaining stability and magnetic tunability [8]. These insights position borophene-based materials as versatile platforms for next-generation 2D superconducting and spintronic devices. ###References 1. Prashant Kumar *et al.*, The rise of borophene, Progress in Materials Science **146**, 101331 (2024). 2. Xiaolong Liu *et al.*, Probing borophene oxidation at the atomic scale, Nanotechnology **33**, 235702 (2022). 3. Qiucheng Li *et al.*, Synthesis of borophane polymorphs through hydrogenation of borophene, Science **371**, 1143-1148 (2021). 4. Caiyun Chen *et al.*, Synthesis of bilayer borophene, Nature Chemistry **14**, 25-31 (2022). 5. Božidar N. Šoškić *et al.*, Enhanced Superconductivity of Hydrogenated β_{12} Borophene, Nano Letters **24**, 12650-12657 (2024). 6. Božidar N. Šoškić *et al.*, First-principles exploration of superconductivity in intercalated bilayer borophene phases, Physical Review Materials **8**, 064803 (2024). 7. Božidar N. Šoškić *et al.*, *Ab-initio* and Monte Carlo study of Fe-based two-dimensional magnets at borophene supported by Ag(111) surface, Physical Review Materials **5**, 074001 (2021). 8. Božidar N. Šoškić *et al.*, Microscopic origin of magnetism in Mn-intercalated bilayer β_{12} borophene - Manuscript in preparation (2025).

Effect of scalar and magnetic impurity on quasiparticle interference of monolayer NbSe$_2$ (16:30, 15 minutes)

Presenter: HANIŠ, Jozef (Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia)

Superconducting transition metal dichalcogenides provide a rich platform for exploring unconventional superconductivity, the spin-orbit coupling effects, and impurity-induced phenomena in two-dimensional systems [1,2,3]. In the talk we discuss the impact of scalar and magnetic single impurities on the quasiparticle interference (QPI) patterns in the superconducting phase of monolayer NbSe$_2$, including the Rashba spin-orbit coupling. We focus on the formation of impurity-bound states, Yu-Shiba-Rusinov states and zero-bias bound states, investigating their signatures in the density of states and their manifestation in QPI patterns. Furthermore, we explore how electron and hole doping modulate the impurity-induced bound states, providing insights into the tunability of impurity physics in 2D superconductors. Exploration of the bound states provides relevant microscopic insight to understanding the impurity effects on unconventional superconductors. ### Acknowledgements This work was supported by the Slovak Research and Development Agency under the Contract no SK-CZ-RD-21-0114, VEGA Grant No.

1/0104/25, Slovak Academy of Sciences project IMPULZ IM-2021-42. ### References [1] J. Haniš, et al., Distinguishing nodal and nonunitary superconductivity in quasiparticle interference of an Ising superconductor with Rashba spin-orbit coupling: The example of NbSe$_2$, Phys. Rev. B **110**, 104502 (2024). [2] D. Sticlet, et al., Topological superconductivity from magnetic impurities on monolayer NbSe$_2$, Phys. Rev. B **100**, 075420 (2019). [3] X. Xi, et al., Ising pairing in superconducting NbSe$_2$ atomic layers, Nat. Phys. **12**, 139 (2016).

time	title	presenter
14:45	Coffee break (30 minutes)	

Friday 23 May 2025

friday morning - Science Technology Park (09:00 - 12:45)

-Conveners: Stavrić, Srdjan (Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade)

Towards Cryo-Spintronics (09:00, 30 minutes)

Presenter: Prof. BLÜGEL, Stefan (Peter Grünberg Institute, Forschungszentrum Jülich)

With the advent of quantum technology and quantum computing, devices at cryogenic temperature become much more wide spread. This also opens opportunities to include superconducting interfaces into the scientific game. For example, the combination of superconductors with magnetic or topological materials offers a playground where new phenomena such as topological superconductivity, Majorana zero modes or superconducting spintronics can emerge. Sofar, superconductivity was mostly investigated on the basis of single s-band models. We changed this providing a materials specific description of complex superconducting heterostructures based on density functional theory by developing the Kohn-Sham Bogoliubov-de Gennes (KS-BdG) method [1] into the Jülich Korringa-Kohn-Rostoker Greenfunction method (juKKR) [2]. By this we turn from a single band model to multiband effects in hybrid structures, which provides a new rich playground for unconventional superconductivity. I will show several examples. One example is the Au/Al heterostructure [3], which allows us to predict finite-energy superconducting pairing due to the interplay of the Rashba surface state of Au, with the hybridization to the electronic structure of superconducting Al. We investigate the nature of the induced superconducting pairing, and we quantify its mixed singlet-triplet character. Our findings demonstrate general recipes to explore real material systems that exhibit interorbital pairing away from the Fermi energy. ### Acknowledgements The work was carried out with Philipp Rüßmann and Björn Trautzettel. Work was supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany’s Excellence Strategy-Cluster of Excellence Matter and Light for Quantum Computing (ML4Q) EXC 2004/1-390534769 and through SFB-1238 (project C1) as well as ERC grant 856538 (project "3D MAGIC"). ### References [1] P. Rüßmann and S. Blügel, Phys. Rev. B 105, 125143 (2022). [2] P. Rüßmann, et al, JuDFTteam/aiida-spirit (2023 [10.5281/ZENODO. 8070769] [3] P. Rüßmann et al., Phys. Rev. Research 5, 043181 (2023).

Orbitronics with magnetic 2D materials (09:30, 30 minutes)

Presenter: MOKROUSOV, Yuriy (Forschungszentrum Jülich)

Orbitronics has recently emerged as a valid alternative to the field of spintronics, with the orbital degree of freedom serving as the main variable for transportation and magnetization manipulation. Currently, the majority of envisioned applications in orbitronics are associated with the generation and utilization of the orbital currents hosted by non-magnetic bulk materials. On the other hand, magnetic two-dimensional (2D) materials are steadily moving to the center of materials research owing to their outstanding properties and prospects in novel magnetic applications. In my talk, I will discuss the interplay of topological features in the electronic structure of 2D magnets with ground-state and current-induced orbital magnetism and orbital currents. Taking as an example selected families of magnetic dichalcogenides, I will demonstrate how the electronic structure engineering of p-d-f hybridization in two dimensions can give rise to prominent topological orbital response, manifesting in the phenomena of current-induced orbital torques on the magnetization and pumping of orbital currents by magnetization dynamics.

Half-Metallic Transport in the Ferromagnetic van der Waals FGT Family (10:00, 15 minutes)

Presenter: NELL, Declan (Trinity College Dublin)

Recent advances in van der Waals (vdW) ferromagnets have opened innovative avenues for spintronic device design. In this work, we present a comprehensive theoretical investigation of coherent spin-dependent transport in the FGT family of vdW ferromagnets. Using density functional theory combined with the non-equilibrium Green's function method, we demonstrate that charge transport perpendicular to the layers exhibits robust half-metallicity driven by its intrinsic electronic structure [1]. Remarkably, this behavior persists from the bulk down to a single layer, remaining resilient under significant bias voltages and in the presence of spin-orbit coupling. We further analyze the tunnel magnetoresistance (TMR) effect in magnetic tunnel junctions composed of various FGT combinations, where the vdW gap serves as the insulating barrier. Notably, a maximum TMR ratio of 800% is achieved in an Fe$_3$GaTe$_2$ bilayer system, and is further enhanced by incorporating additional layers. Expanding our study to include dynamical effects via an extended dynamical mean field theory approach [2], we examine the influence of electronic correlations in Fe$_4$GeTe$_2$. While transport remains largely coherent at low bias, above ~0.5 V, spin-down Fe $3d$ states enter the bias window, triggering inelastic scattering and destroying coherence. This results in broadened spectral features and enhanced density of states near the Fermi level. A current decomposition confirms a growing incoherent contribution beyond this threshold. ### References [1] A. Halder, D. Nell, A. Sihi, A. Bajaj, S. Sanvito, and A. Droghetti, Half-Metallic Transport and Spin-Polarized Tunneling through the van der Waals Ferromagnet Fe4GeTe2, Nano Lett. 24, 9221 (2024). [2] D. Nell, S. Sanvito, I. Rungger, and A. Droghetti, Effect of dynamical electron correlations on the tunnelling magnetoresistance of Fe/MgO/Fe(001) junctions, Phys. Rev. B 111, (2025).

Strain-tuning of spin anisotropy in single-layer phosphorene: insights from Elliott-Yafet and Dyakonov-Perel spin relaxation (10:15, 15 minutes)

Presenter: JURECZKO, Paulina (Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 04001 Košice, Slovakia, Institute of Physics, University of Silesia in Katowice, 41-500 Chorzów, Poland)

Persistent spin textures give rise to robust spin states, unlocking wide-range opportunities for quantum computing, data storage, and advanced spintronic technologies [1]. In this work, we explore the potential for realizing a persistent spin texture in monolayer phosphorene - a promising spintronic material with high carrier mobility, tunable semiconducting band gap and weak spin-orbit coupling [2,3]. Using first-principles calculations, we investigate the effects of strain and external transverse electric field on spin anisotropy in phosphorene bands. Strain is varied from -5% to +5% along zigzag and armchair directions across different electric field strengths. We find that while strain applied along the armchair direction has a minor effect on spin physics, strain along the zigzag direction leads to qualitative changes in spin anisotropy. In particular, for 1.2% strain in the zigzag direction, a persistent spin texture, with spins polarized in the x-direction, appears in the conduction band of phosphorene, even for arbitrarily small electric fields. In effect, spin relaxation triggered by the Dyakonov-Perel [4] spin relaxation mechanism is effectively deactivated for S$_x$ spins. The analysis of intrinsic spin-orbit coupling by the spin-mixing parameter b^2 [5] reveals that tensile strain has a minor impact of up to 4%, with the anisotropy ratio reaching 2. For 5%, the anisotropy sharply rises to 100, driven by band anticrossing and evolving with doping. In zero-electric field case with preserved inversion symmetry, the Elliott-Yafet mechanism dominates the spin relaxation process. Our findings highlight that tuning the strain in the phosphorene enables an excellent platform for manipulating the spin texture or spin anisotropy, simultaneously enhancing the spin lifetime [6]. ###Acknowledgement The authors acknowledge financial support from NCBR under the V4-Japan project BGapEng V4-JAPAN/2/46/BGapEng/2022 and ICM UW, within grant no. G83-27 and Slovak Academy of Sciences project IMPULZ IM-2021-42. ###References [1] L. L. Tao and E. Y. Tsymbal, Persistent spin texture enforced by symmetry, Nat. Commun. 9, 2763 (2018). [2] L. Cording, J. Liu, J. Y. Tan, et al., Highly anisotropic spin transport in ultrathin black phosphorus, Nat. Mater. 23, 479 (2024). [3] H. Liu, A. T. Neal, Z. Zhu, Z. Luo, X. Xu, D. Tománek, and P. D. Ye, Phosphorene: An unexplored 2D semiconductor with a high hole mobility, ACS Nano 8, 4033 (2014). [4] M. I. Dyakonov and V. I. Perel, Spin relaxation of conduction electrons in noncentrosymmetric semiconductors, Sov. Phys. Solid State 13, 3023 (1971). [5] B. Zimmermann, P. Mavropoulos, S. Heers, N. H. Long, S. Blügel, and Y. Mokrousov, Anisotropy of spin relaxation in metals, Phys. Rev. Lett. 109, 236603 (2012). [6] P. Jureczko, M. Milivojević, and M. Kurpas, Strain-tuning of spin anisotropy in single-layer phosphorene: Insights from Elliott-Yafet and Dyakonov-Perel spin relaxation rates, arXiv:2501.05911 (2025).

Prospects for increasing the Curie temperature in monolayer $ {\rm CrI_3}$ by carrier doping (11:00, 15 minutes)

Presenter: OROZOVIĆ, Marko (Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade)

The discovery of ferromagnetism in monolayer ${\rm CrI_3}$ marked the beginning of a new era in two-dimensional (2D) materials research. However, most 2D ferromagnets exhibit critically low ordering temperatures, limiting their technological applicability [1]. Significant efforts have focused on enhancing the modest Curie temperature (T_c) of monolayer ${\rm CrI_3}$ (45 K), with carrier doping emerging as a particularly promising strategy [2]. Theoretical studies suggest that electron or hole doping could elevate T_c to values up to five times higher than the experimental one [3]. Yet, the orbital-resolved mechanisms governing the evolution of superexchange interactions in doped systems remain poorly understood. In this theoretical study, we combine ab initio density functional theory (DFT), spin Hamiltonian modeling, and Wannier function analysis to systematically investigate doping-dependent magnetic interactions in monolayer ${\rm CrI_3}$. By decomposing superexchange pathways into orbital-specific contributions from Cr and I atoms, we correlate shifts in orbital occupancy with changes in magnetic coupling strength. Hole doping suppresses $t_{2g}-t_{2g}$ antiferromagnetic coupling while maintaining ferromagnetic $t_{2g}-e_g$ interaction. In contrast, for electron doping, the enhancement of ferromagnetic e_g-e_g coupling is compensated by a decrease in $t_{2g}-e_g$ interaction. As a result, hole doping proves to be a more effective strategy for increasing T_c. Furthermore, we investigate the doping-dependent evolution of spin-orbit coupling (SOC)-driven magnetic interactions. Notably, the Dzyaloshinskii-Moriya interaction (DMI) between the second-nearest neighbors remains unchanged under electron doping but increases dramatically with hole doping, reaching 110% ratio in D/J_2 at one hole per unit cell. Most critically, we show that this pronounced DMI enhancement counteracts the rise in T_c, leaving it nearly unaltered across a broad doping range. Our work identifies DMI as a key limiting factor for T_c enhancement in carrier-doped ${\rm CrI_3}$, underscoring its essential role in the design of functional 2D magnets. ### References [1] B. Zhang et al., npj Spintronics **2**, 6 (2024). [2] S. Jiang et al., Nature Nanotech **13**, 549–553 (2018). [3] C. K. Singh et al., Phys. Rev. B **103**, 214411 (2021). [4] M. Orozović, B. Šoškić, Ž. Šljivančanin, S. Stavrić, Prospects for increasing the Curie temperature in monolyer CrI3 by carrier doping - manuscript in preparation.

Magnetic properties and electronic response of monolayer α-NbSi$_2$N$_4$ (11:15, 15 minutes)

Presenter: MOŠKO, Timon (Pavol Jozef Šafárik University in Košice, Faculty of Science, Institute of Physics)

The recently discovered group of intercalated monolayers with structural formula MA$_2$Z$_4$ attracted significant interest due to the wide range of physical properties [1]. In the talk we discuss the α-NbSi$_2$N$_4$ monolayer as a two-dimensional ferromagnet with promising magnetic, thermal and optical properties for future spintronics applications. Specifically, using density

functional theory (DFT) we study mechanical stability and possibility of charge density waves formation. We examine the dielectric properties within the Random Phase Approximation [2] and discuss the effect of the overlap matrix elements and constant matrix element approximation on electronic susceptibility. Optical conductivity based on the Berry curvature calculations, and orbital magnetization were analyzed using an effective model with a localized Wannier basis. The magnetic properties were studied within the classical Heisenberg model with a uniaxial anisotropy term. The model parameters were determined by mapping the total electronic energy for different magnetic configurations to the model. Magnon dispersions and Curie temperature using Monte Carlo simulations are discussed. ### Acknowledgements This work was supported by the Slovak Research and Development Agency under the Contract no. SK-SRB-23-0033, VEGA Grant No. 1/0104/25, Slovak Academy of Sciences project IMPULZ IM-2021-42. ### References [1] L. Wang et al., Intercalated architecture of MA$_2$Z$_4$ family layered van der Waals materials with emerging topological, magnetic and superconducting properties, Nature Comm. 12, (2021). [2] J. Sólyom, Fundamentals of the Physics of Solids (Springer Berlin Heidelberg, 2010).

Proximity-Induced Magnetic Phases in CrI□ Monolayers Coupled to WSe□ (11:30, 15 minutes)

Presenter: TAJKOV, Zoltán (Eötvös Loránd University)

We investigate the emergence of altered magnetic phases in a CrI□ monolayer induced by proximity effects with WSe□. Using density functional theory (DFT) calculations within the SIESTA framework, we analyze the magnetic properties via a novel approach for extracting the magnetic exchange interaction and onsite anisotropy tensors in extended Heisenberg spin models, explicitly incorporating relativistic effects. This method, based on the Liechtenstein-Katsnelson-Antropov-Gubanov torque formalism, evaluates energy variations upon infinitesimal spin rotations. Our results provide insight into how a 2D magnet is influenced when coupled to a material with strong spin-orbit coupling. Additionally, we explore the impact of varying twist angles, considering the incommensurability of the CrI□ and WSe□ unit cells.

Switching of the magnetic anisotropy in hole-doped H-VTe$_2$ by spin-orbit splitting (11:45, 15 minutes)

Presenter: EUSTE, John Lawrence (The Abdus Salam International Centre for Theoretical Physics (ICTP) & Scuola Internazionale Superiore di Studi Avanzati (SISSA))

The H-phase of vanadium ditelluride (H-VTe$_2$) recently gained interest in spintronics due to its room-temperature ferromagnetism and tunable electronic band gap [1]. The stability of its ferromagnetic ordering in the monolayer structure can be attributed to its large magnetic anisotropy energy (MAE), favoring in-plane magnetization. Modulating the magnetic anisotropy is crucial in improving low-dimensional spintronic devices; one of the effective methods to achieve this is through electrostatic doping [2]. Yet, the underlying mechanism driving the changes in MAE upon doping is still unclear. We performed a density functional theory study to determine the effect of electrostatic doping on the electronic and magnetic properties of H-VTe$_2$ monolayer. Our calculations revealed that hole doping increases the magnitude of MAE in the order of millielectronvolts, switching the magnetic anisotropy to easy out-of-plane magnetization even for small doping concentrations. We found that the interplay of orbital hybridization, exchange splitting, and crystal field splitting from the trigonal prismatic coordination pushes a two-fold degenerate d_{xz}/d_{yz} state to the valence band edge at Γ. The energy splitting of this doublet due to SOC is crucial in lowering the fully relativistic total energy of the system upon hole doping when the magnetization axis is perpendicular to the surface. Aside from the switching of MAE, we found that hole doping induces a semiconductor to half-metal transition and enhances the magnetic moment, which makes H-VTe$_2$ a promising material for spintronics application. The proposed mechanism for the influence of electrostatic doping on MAE can also apply to other systems where spin-orbit coupling affects states near the Fermi level. ### References [1] M. Jafari, W. Rudziński, J. Barnaś, and A. Dyrdał, Electronic and magnetic properties of 2D vanadium-based transition metal dichalcogenides, Sci Rep **13**, (2023). [2] R. Han, X. Xue, and Y. Yan, Hole-Doping-Induced Perpendicular Magnetic Anisotropy and High Curie Temperature in a CrSX (X = Cl, Br, I) Semiconductor Monolayer, Nanomaterials **13**, 3105 (2023).

AMaRaNTA: An AiiDA-based Workflow To Automate Calculations Of Exchange Parameters In 2D Magnets (12:00, 15 minutes)

Presenter: ORLANDO, Federico (Politecnico di Milano, Milan (Italy))

2D magnetic materials have sourced great attention in the last few years [1]. Intrinsic theoretical interest arises from the very existence of magnetism below the 3D limit, proven only recently after decades of debate, as well as from the observed richness in magnetic phases, encompassing conventional ferromagnetic and antiferromagnetic as well as more exotic textures. Besides, these materials are known to offer practical applications in fields such as spintronics. The popularity gained by such research field has driven the adaptation of first-principles approaches, combined with model Hamiltonians, to calculate exchange parameters, crucial for the prediction of magnetic textures [2]. However, the methodology is not uniquely established as of today, which results in a lack of systematicity in the data produced; as a consequence, inhomogeneous and/or incomplete predictions may arise, preventing a full comprehension of the nature of exchange interaction in some cases [3]. To address such issue, we present AMaRaNTA (Automating MAgnetic paRAmeters iN a Tensorial Approach), a computational package that systematically automates Density Functional Theory (DFT) simulations of exchange parameters for 2D magnets. Within AMaRaNTA, these are characterized by means of a nearest-neighbour exchange tensor, along with scalar parameters for the second- and third-neighbour exchange and the single-ion anisotropy. Both aspects allow us to push the research beyond the state of the art,

since previous efforts in this respect were limited to nearest neighbours and partially-tensorial approaches only [4]. As of today, we have already employed AMaRaNTA to prepare a compact database of exchange parameters for around 30 materials [5]. AMaRaNTA comes in the form of an AiiDA workchain [6], based on the Vienna Ab-initio Simulation Package (VASP) for DFT calculations [7]; actual evaluation of the exchange parameters is done by post-processing DFT total energies via the so-called four-states method [2]. Ease of use is guaranteed in that the user is only required to provide a structure file; AMaRaNTA takes care of building the necessary simulation cells and, through AiiDA, to set up all calculations, retrieve the results and extract the exchange parameters. ### References [1] M. Gibertini et al., Nat. Nanotechnol. **14**, 408 (2019). [2] X. Li et al., Molecules **26**, 803 (2021). [3] J.Y. Ni et al., Phys. Rev. Lett. **127**, 247204 (2021). [4] D. Torelli et al., npj Comput. Mater. **6**, 158 (2020). [5] F. Orlando et al. (manuscript in preparation). [6] G. Pizzi et al., Computational Materials Science, **111**, 218 (2016). [7] G. Kresse and J. Furthmüller, Phys. Rev. B 54, 11169 (1996)

ML based approach for calculating the dynamics of sulfur vacancies in monolayer MoS$_2$: extensive study (12:15, 15 minutes)

Presenter: HLOŽNÝ, Adam (Slovak Academy of Sciences)

We have developed a multi-step strategy for training stable and precise machine learning potentials (MLPs) that are able to efficiently and precisely extrapolate to out-of-domain (OOD) cases. Essential part of obtaining well-performing MLP is obtaining balanced and properly sampled dataset. To achieve this, we have developed a sampling technique based on nudged elastic band (NEB) and constrained molecular dynamics. We demonstrate the utility of our approach by calculating properties of (multi-)vacancies in MoS$_{2}$ monolayer such as structural relaxations, minimum energy paths, barriers and temperature-dependent free energy barriers. We evaluate precision of the model to great detail to find it's limitations in various cases. Usually, MLPs are evaluated using metrics such as RMSE on all the data and all the atoms at once, however, this does not show the full picture, since the most interesting configurations, such as those close to the transition states, are usually the ones with the highest error. We performed an extensive benchmarking of the MACE model in the context of vacancy dynamics in monolayer MoS$_{2}$ and checked the behavior of the model in most extreme cases for atoms close to the vacancy and in near-barrier configurations, which are the most difficult for the model to reproduce. Generally, we found that the MACE model is able to sufficiently reproduce energies and forces even in these extreme cases. We believe our conclusions are also valid for other symmetry-based *message passing neural network* potentials due to their general similarity.

Exploring the magnetic landscape of easily-exfoliable two-dimensional materials (12:30, 15 minutes)

Presenter: HADDADI, Fatemeh (EPFL, Switzerland)

Magnetic materials often exhibit complex energy landscapes with multiple local minima, each corresponding to a self-consistent electronic structure solution. Finding the global minimum is challenging, and heuristic methods are not always guaranteed to succeed. We apply an automated workflow to systematically explore the energy landscape of 194 magnetic monolayers from the Materials Cloud 2D crystals database and determine their ground-state magnetic order. Our approach enables effective control and sampling of orbital occupation matrices, allowing rapid identification of local minima. We reveal a diverse set of self-consistent collinear metastable states, further enriched by Hubbard-corrected energy functionals with U parameters computed from first principles using linear response theory. We categorize the monolayers by their magnetic ordering and highlight promising candidates for applications. Our results include 107 ferromagnetic, 85 antiferromagnetic, and 2 altermagnetic monolayers.

time	title	presenter
10:30	Coffee break (30 minutes)	

Worskhop closing - Science Technology Park (12:45 - 13:00)