HL 5: 2D Materials: Electronic structure, excitations, etc. I (joint session O/HL/TT)

Time: Monday 10:30–12:30 Location: TRE/MATH

Invited Talk HL 5.1 Mon 10:30 TRE/MATH

Magnetic Order in 2D Materials Beyond Bulk Constraints — •Jeison Fischer — II. Physikalisches Institut, Universität zu Köln

Even though exfoliated microflakes remain widely used in 2D magnetism research, their bulk origin restricts access to many potentially interesting phases, an obstacle that molecular beam epitaxy (MBE) can overcome. MBE enables the controlled synthesis of single-layer materials directly related to, yet often distinct from, their bulk counterparts.

In my talk, I will present structural characterization and discuss the mechanisms behind the formation of such novel 2D materials grown via MBE on graphene. [1-2] The emerging magnetic properties of these new 2D materials will be exemplified with two cases: Cr_2S_3-2D and Fe_2S_2-2D. Cr_2S_3 forms a covalently bonded NiAs-type structure without van der Waals gaps. Using spin-polarized scanning tunneling microscopy (STM) and X-ray magnetic circular dichroism (XMCD), we show that it hosts ferromagnetic coupling within the plane with magnetic moments pointing out-of-plane, combined with A-type antiferromagnetic coupling between different Cr planes. Fe_2S_2 exhibits a unique hexagonal phase, in which Fe atoms occupy tetragonally coordinated sites. Spin-polarized STM reveals that the moments are noncollinear within the plane. We map the in-plane components of two distinct magnetic configurations and find that the moments are confined to the 2D plane, forming a Néel state and a 2Q state.

[1] Knispel et al. Small, 2025 21, 2408044.
[2] Safeer et al. Adv. Funct. Mater. 2025, 202500907.

HL 5.2 Mon 11:00 TRE/MATH

Ab initio modeling of magnons and magnon-phonon coupling in 2D magnetic materials — Ali Esquembre-Kucukalic1[1], Khoa Le[2], Hsiao-Yi Chen[3], Ivan Maliyov[2], Jin-Jian Zhou[4], Davide Sangalli[5], and •Alejandro Molina-Sánchez[1] — [1]ICMUV, University of Valencia, Valencia, Spain — [2]CALTECH, California, USA — [3]Tohoku University, Japan — [4]Beijing Institute of Technology, Beijing, China — [5]ISM-CNR, Roma, Italy

Understanding spin-wave excitations in two-dimensional magnetic materials is essential for advancing spintronic and quantum information technologies. Chromium trihalides and related 2D magnets provide a platform where the choice of halide influences on the magnetic behavior, yet its impact on magnon properties is not completely understood. We present first-principles calculations of magnon dispersions and wave functions in monolayer Cr trihalides using the Bethe-Salpeter equation (BSE), resolving key features such as the topological gap at the Dirac point. The BSE analysis reveals that magnons originate from electronic transitions spanning a wider energy range than excitons, offering new insight magnon character and enabling the extraction of Heisenberg exchange parameters. Building on this framework, we develop an ab initio description of mag-ph coupling by deriving BSE-based mag-ph interaction matrices and applying them to monolayer CrI3 and hydrogenated graphene. We show that mag-ph and electron-phonon couplings differ markedly, identifying specific phonon modes that dominate magnon scattering.

HL 5.3 Mon 11:15 TRE/MATH

Electron-phonon interaction in transition-metal dichalcogenides — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial effect in solid state physics, in particular in two-dimensional materials. We developed a generally applicable ab-initio implementation on top of density functional theory using a basis set of localized Gaussian orbitals. It combines finite differences calculations with the perturbative Allen-Heine-Cardona framework in order to calculate the temperature-dependent renormalization of the electronic bandstructure due to electron-phonon interaction. Our implementation circumvents the limiting problems of previous implementations and allows to evaluate Debye-Waller contributions beyond the rigid-ion approximation [1], which are usually neglected.

In addition to the renormalization of the electronic bands, electron-phonon interaction introduces a line broadening due to finite-lifetime effects, which have recently been incorporated into our implementation. In this presentation, we discuss our results, including those with finite-lifetime effects, for two-dimensional transition-metal dichalcogenides, where the renormalization of the electronic bandstructure due to electron-phonon interaction can be as large as several hundreds of meV.

[1] Mann et al., Phys. Rev. B **110**, 075145 (2024)

HL 5.4 Mon 11:30 TRE/MATH

Surface-state engineering for nonlinear charge and spin photocurrent generation — •Javier Sivianes[1], Peio Garcia-Goiricelaya[2], Daniel Hernangómez-Pérez[3], and Julen Ibañez-Azpiroz[1,4,5] — [1]Centro de Física de Materiales (CSIC-UPV/EHU), Donostia, Spain — [2]University of the Basque Country UPV/EHU, Leioa, Spain — [3]CIC nanoGUNE BRTA, San Sebastián, Spain — [4]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [5]Donostia International Physics Center (DIPC), Donostia, Spain

We systematically explore the generation of nonlinear charge and spin photocurrents using spin-orbit-split surface states. This mechanism enables net DC flow along the surface plane even in centrosymmetric bulk environments like the Rashba prototype Au(111), where we characterize the main quadratic contributions by combining model predictions with density functional calculations. We further identify the Tl/Si(111) surface as a prime scenario for experimental verification; with slight doping, it develops metallic surface states featuring remarkable relativistic properties deviating from the Rashba paradigm, while the bulk remains semiconducting. Its nonlinear charge photocurrent reveals a distinct angular signature and a magnitude comparable to bulk ferroelectrics, highlighting the potential of surface-state photocurrents for low-bias optoelectronic applications. Moreover, the nontrivial spin texture of its surface states enables the generation of pure out-of-plane spin-polarized currents, offering a highly versatile nonlinear spin-filtering functionality beyond the conventional spin Hall effect.

HL 5.5 Mon 11:45 TRE/MATH

Influence of Vanadium Doping on WSe_2, as seen through ARPES — •Jana Kähler[1,2], Florian K. Diekmann[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Adina Timm[1,2], Anja Yalim[1,2], Jens Buck[1,2], Meng-Jie Huang[2], Jules M. Knebusch[1,2], Luka Hansen[1,3], Jan Benedikt[1,3], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics offers a compelling, energy-efficient alternative to traditional electronics with potential applications in communications, sensing, and information processing. The vanadium-doped layered transition metal dichalcogenide 2*H*-WSe_2 is particularly promising as a room-temperature magnetic semiconductor with gate-tunable transport properties. Here, we use a combination of 11 eV laser, 21.2 eV He-lamp, and soft X-ray synchrotron ARPES to highlight the influence of a fairly small vanadium doping on the electronic structure of WSe_2. Both the pristine and doped compounds were grown by chemical vapor transport in our own laboratory.

HL 5.6 Mon 12:00 TRE/MATH

Engineering sulfur vacancy dimers in monolayer WS_2 — •Daniel Jansen[1], Guangyao Miao[1], Jan Keienburg[1], Jeison Fischer[1], Thomas Michely[1], Hannu-Pekka Komsa[2], and Wouter Jolie[1] — [1]Institute of Physics II, University of Cologne, Cologne, Germany — [2]Faculty of Information Technology and Electrical Engineering, University of Oulu, Oulu, Finland

Sulfur vacancies [1] and sulfur vacancy dimers in nearest-neighbor distance [2] in monolayer WS_2 have been experimentally proven to yield bright and stable photon emission, thus holding promises for the development of quantum technologies.
Here we investigate dimers of sulfur vacancies in different configurations in monolayer WS_2 created with the tip of a scanning tunneling microscope [3]. Scanning tunneling spectroscopy reveals strong hybridization of the sulfur vacancy electronic in-gap states, validated by density functional theory calculations. For dimers in nearest-neighbor configuration we find that inelastically tunneling electrons can induce sulfur atom migration, resulting in a rotary motion of the dimer. This

motion is studied in detail by analyzing the emerging telegraph noise in the junction. Lastly, we elaborate on scenarios to make use of the dimer motion for the design of vacancy structures and lattices.

[1] Schuler et al., Sci. Adv. **6**, 38 (2020)
[2] Sun et al., Nature Commun. **15**, 9476 (2024)
[3] Jansen et al., Phys. Rev. B **109**, 195430 (2024)

HL 5.7 Mon 12:15 TRE/MATH

Alkali-metal doped transition metal chlorides confined in bilayer graphene: Insights from first-principles calculations — •Munawar Ali[1], Arkady V. Krasheninnikov[2], Giovanni Cantele[1], and Mahdi Ghorbani-Asl[2] — [1]Università degli Studi di Napoli "Federico II," Dipartimento di Fisica "Ettore Pancini," Complesso di Monte S. Angelo, via Cinthia, 80126 Napoli, Italy — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

The intercalation of atomic and molecular species into layered materials has emerged as a powerful strategy for synthesizing novel two-dimensional systems with tunable electronic, magnetic, and energy-storage properties. Encapsulating transition-metal halides into bilayer graphene has proven effective for stabilizing 2D magnetic phases that are otherwise thermodynamically unstable. Using density functional theory, we systematically investigate the intercalation of metal chlorides (TCl_3, T = Fe, Cu, Mo, Al) doped with alkali metals (Li, Na, K, Rb, Cs) across a range of concentrations. Li- and Na-doped $FeCl_3$, $CuCl_3$, and $MoCl_3$ monolayers exhibit the highest thermodynamic stability, whereas $AlCl_3$ remains unstable even under doping. Bader charge analyses reveal substantial charge transfer from the graphene host to the intercalated layers, particularly in the case of $CuCl_3$, which also shows the strongest binding. These findings provide a theoretical framework for understanding the stability of these heterostructures and highlight alkali-metal-intercalated graphene systems as a platform for engineering tunable 2D magnetic materials.