HL 39: 2D semiconductors VII – CrSBr and related heterostructures

Time: Thursday 9:30–12:30 Location: POT/0081

HL 39.1 Thu 9:30 POT/0081

Ab initio investigation of electronic, magnetic, optical properties and proximity effect in MoS_2/CrSBr van der Waals heterostructures — •Athanasios Koliogiorgos and Karel Carva — Charles University, Prague, Czech Republic

CrSBr-MoS_2 heterostructures combine the properties of the antiferromagnetic semiconductor CrSBr and the TMD semiconductor MoS_2, yielding a promising platform for spintronic and valleytronic applications. In connection with experimental work, using density functional theory with GGA+U and hybrid HSE06 functionals, we explore the structural, electronic, magnetic and optical properties of MoS_2/CrSBr systems, where CrSBr is 1-4 layers thick and MoS_2 a monolayer. We observe induced magnetization in the MoS_2 layer via proximity effect, strongly dependent on the interlayer distance. Other proximity effects include charge transfer, bandgap renormalization and spin splitting in the band structure, while the density of states reveals a weakly hybridized system, retaining the characteristics of the separate parts. Work function and band alignment show that the material behaves as a Type-II heterostructure. The calculation of the absorption coefficient reveals distinct peaks corresponding to the CrSBr and MoS_2 layers, in agreement with the experimental photoluminescence spectrum.

HL 39.2 Thu 9:45 POT/0081

Proximity-Induced Raman Signatures in a $NbSe_2$-CrSBr Superconductor-Magnet Heterostructure — •Elena Vinnemeier[1], Jan-Hendrik Larusch[1], Kai Rossnagel[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany

Interfacing superconducting $NbSe_2$ with the antiferromagnetic semiconductor CrSBr provides a van der Waals platform to study proximity effects in quantum devices. The superconductivity-magnetism interplay enables Josephson junctions and superconducting quantum interference devices with field-tunable critical current and spin filtering. We study proximity effects of the spin ordered CrSBr on the specific collective modes in $NbSe_2$ in the superconducting phase at 4K and the charge-density wave phase at 15K. A magnetic field tunes CrSBr from antiferromagnetic to ferromagnetic order. The Raman response of the heterointerface, relative to bare $NbSe_2$, reveals proximity effects from the ferromagnetic CrSBr layer at the interface. Modifications of the $NbSe_2$ collective excitation spectrum demonstrate strong interaction between the proximitized magnetic order in CrSBr and correlated phases in $NbSe_2$. This project was supported by the EIC pathfinder grant 101130224 "JOSEPHINE".

HL 39.3 Thu 10:00 POT/0081

Exciton dominated anisotropic dielectric tensor in CrSBr — •Jan-Hendrik Larusch[1], Pierre-Maurice Piel[1], Aleksandra Łopion[1], Thomas Kliewer[1], Zdeněk Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

CrSBr is an air-stable magnetic vdW semiconductor with a direct bandgap; its anisotropic spin, lattice, and charge, drive anisotropic light-matter interaction $\varepsilon(\omega)$. We directly determine the full dielectric tensor of exfoliated CrSBr by spectroscopic imaging ellipsometry (SIE). In the paramagnetic phase, SIE verifies $\varepsilon_{xx} \times \varepsilon_{yy} \times \varepsilon_{zz}$. Room-temperature comparison of Mueller-matrix and generalized ellipsometry guides cryogenic SIE, enabling us to track changes across the Curie and Néel temperatures as the system evolves from paramagnetic over intralayer ferromagnetism to A-type antiferromagnetism. In the AFM phase, polarization-resolved magneto-reflectance with fields along c (hard), b (easy), and a (intermediate) axis yields critical fields of roughly 2.2, 1.05, and 0.3 T for transition to FM order sensed by distinct optical fingerprints. Together, these measurements quantify the anisotropic light-matter interaction and its dependence on magnetic order, linking exciton-dominated emission/absorption to the full dielectric tensor [1]. [1] J. Klein et al. ACS Nano 17, 5316-5328 (2023).

HL 39.4 Thu 10:15 POT/0081

Optical Probing of Interfacial Magnetic Properties of the CrSBr-$MnPS_3$ hetero-interface — •Thomas Kliewer[1], Aleksandra Łopion[1], Pierre-Maurice Piel[1], Jan-Hendrik Larusch[1], Zdeněk Sofer[2], and Ursula Wurstbauer[1] — [1]University of Münster, Germany — [2]University of Chemistry and Technology Prague, Czech Republic

CrSBr and $MnPS_3$ are both 2D antiferromagnetic semiconductors with different magnetic and optical properties. $MnPS_3$ has out-of-plane spin alignment while CrSBr's spins are aligned in-plane [1,2]. Interfacing these two materials is expected to result in complex interfacial spin-alignment, presumably with the stabilization of a non-collinear magnetic phase at the interface. CrSBr exhibits strong excitonic features coupled to the magnetic order [3]. This is used as a probe for the magnetic situation of the $MnPS_3$-CrSBr interface. The structures are characterized by polarization-resolved Raman spectroscopy measurements and the interfacial magnetic properties are probed by low-temperature magneto-photoluminescence and reflectance spectroscopies. We observed a peculiar influence of $MnPS_3$ on the optical response of CrSBr. A proximity-induced modification of the magnetic properties of CrSBr interfaced with $MnPS_3$ seems to induce long-range order, since the impact is observable on the CrSBr flake more than 10 μm away from the interfaced region. Our observations might be connected to the stabilization of an intermediate ordered magnetic state in CrSBr. [1] Wilson, et al. Nat. Mat. 20.12 (2021), [2] Kobets, et al. Low Temp. Phys. 35.12 (2009), [3] Heißenbüttel, et al. Phys. Rev. B 111.7 (2025)

HL 39.5 Thu 10:30 POT/0081

Coupling Between Vibrational, Electronic, and Magnetic States in CrSBr — •Daria Markina[1], Priyanka Mondal[1], Lukas Krelle[1], Sai Shradha[1], Mikhail M. Glazov[2], Regine von Klitzing[1], Kseniia Mosina[3], Zdenek Sofer[3], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]St. Petersburg, Russia — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic

The van der Waals antiferromagnet CrSBr displays interplay between vibrational, electronic, and magnetic states, producing distinctive quasiparticle interactions. Using temperature-dependent polarization-resolved Raman spectroscopy with optical absorption and photoluminescence excitation (PLE), we examine these effects across the magnetic phase transition. Under 1.96 eV excitation, the A_g^1, A_g^2, and A_g^3 Raman modes exhibit pronounced polarization and intensity changes near the Néel temperature, accompanied by modifications in excitonic oscillator strength and resonant PLE features. The distinct temperature evolution of Raman tensor elements indicates that individual phonons couple to specific excitonic and electronic states. The suppression of excitonic transitions above the Néel temperature links these effects to spin alignment, suggesting an indirect spin−phonon interaction mediated by exciton−phonon coupling. These findings establish CrSBr as a promising platform for studying quasiparticles in two-dimensional magnets and for potential quantum technologies.

HL 39.6 Thu 10:45 POT/0081

Evidence for a novel spin-density excitation in 2D magnetic semiconductor CrSBr — •Pierre-Maurice Piel[1], Jan-Hendrik Larusch[1], Aleksandra Łopion[1], Zdenek Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

The van der Waals magnet CrSBr is an air-stable semiconductor with ferromagnetic layers, antiferromagnetic interlayer coupling, and a highly anisotropic bandstructure, resulting in quasi-one-dimensional excitonic states [1]. We probe the impact of magnetic order on excitons and collective modes using low temperature (4K) magneto photoluminescence and resonant Raman spectroscopy with special emphasize on the magnetic anisotropy and magnetic phase transitions. The excitonic signatures in photoluminesence show clear differences between antiferromagnetic and ferromagnetic regimes and reveal pronounced magnetic anisotropy. In resonant Raman, the first order Ag phonons remain essentially field independent, whereas additional modes appear only under excitonic resonance. We resolve a sharp mode near 248 cm-1 emerging in resonance with the A-exciton (~1.36eV) and a broad mode at 362 cm-1 occurring in A and higher-lying excitonic regimes.

The mode's excitation energy and field dependence indicate selective access to different collective possibly spin-density excitations in CrSBr. [1] J. Klein et al., ACS Nano 17, 5316-5328 (2023).

15 min. break

HL 39.7 Thu 11:15 POT/0081

Tracking Magnetic Phase Evolution in CrSBr via Excitonic Emission and Absorption — •Lukas Krelle[1], Ryan Tan[1], Daria Markina[1], Priyanka Mondal[1], Kseniia Mosina[2], Kevin Hagmann[1], Regine von Klitzing[1], Zdenek Sofer[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic

CrSBr is an air-stable magnetic van der Waals semiconductor, in which the interaction of excitons with the magnetic order enables the optical identification of different magnetic phases. Here, we study multi-layer samples of CrSBr inside a three-axis vector magnet and correlate magnetic order and optical transitions. We identify layer by layer switching of the magnetization through drastic changes of the optical absorption energy and strength as a function of the applied magnetic field. We find that ferromagnetic and antiferromagnetic order between layers can coexist in the same domain [1]. The photoluminescence evolution depends on the magnetic order and can differ for each emission. The intensity of energetically lower lying transitions reduces monotonously with increasing field strength whereas energetically higher lying transitions around the bright exciton increase in intensity close to the saturation field. Using this contrasting behavior we can therefore correlate transitions with each other. [1]: L. Krelle et al, ACS Nano 2025, 19, 33156

HL 39.8 Thu 11:30 POT/0081

Magnetically controllable exciton-polariton condensation in CrSBr microwires — •Christian Weidgans[1], Heng Zhang[1], Niloufar Nilforoushan[1,4], Julian Hirschmann[2], Marlene Liebich[1], Tobias Inzenhofer[1], Imke Gronwald[1], Josef Riepl[1], Kseniia Mosina[3], Zdeněk Sofer[3], Fabian Mooshammer[1], Florian Dirnberger[2], and Rupert Huber[1] — [1]University of Regensburg, Germany — [2]Technical University of Munich, Germany — [3]University of Chemistry and Technology Prague, Czech Republic — [4]Université Paris Cité, France

Coupling the macroscopic wave functions of quasiparticle condensates to other degrees of freedom, such as the electron spin, could offer valuable control knobs for future quantum applications. In particular, man-made condensates of light-matter hybrids known as exciton-polaritons have lacked a direct spin-related control mechanism. Here we demonstrate magnetically tunable exciton-polariton condensation in the antiferromagnetic semiconductor CrSBr, a van der Waals material with strongly linked optical and magnetic properties. Under photoexcitation, CrSBr microwires embedded in an optical cavity show the hallmarks of polariton condensation. The conditions for efficient optical pumping suggest a crucial role of recently discovered surface excitons. Applying an external magnetic field energetically shifts the photoemitting polariton states, enabling direct spin-based control. Our results highlight CrSBr microwires as a powerful platform for exploring magnetically tunable polariton condensates, their directional propagation and their potential for spin-based quantum devices.

HL 39.9 Thu 11:45 POT/0081

Preparation and characterization of CrSBr on opal substrtates — •Jannik Schürmann[1], Aleksandra Lopion[1], Ursula Wurstbauer[1], Alexey V. Scherbakov[2], and Giulia Magnabosco[3] — [1]University of Münster, Münster, Germany — [2]Technische Universität Dortmund, Dortmund, Germany — [3]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

The magnetic semiconductor Chromium-Sulfur-Bromide (CrSBr) is a highly anistropic van der Waals material. To study the anisotropy of the phononic properties independent from the supporting substrate, the flakes can be detached from it either by suspending it over cavities or by transferring it to a substrate containing closely packed silica spheres (opals). This second approach was already applied to other, nonmagnetic vdW materials such as WSe2 allowing an in-depth pump-probe study of phonons in the material [1]. Accordingly, we transfer mechanically exfoliated CrSBr onto opal substrates using polycarbonate stamps (dry transfer) and thoroughly characterize the properties and qualities of the flakes on opals. Atomic force microscopy confirms that CrSBr is on top of the spheres and partially freestanding. PL and Raman measurements are performed to validate the behavior of the flake in comparison with fully supported one. The decoupled CrSBr flakes on opal substrates are suitable for pump-probe studies of phonon states in CrSBr.

[1] A. Carr et al, ACS Photonics, 11, 1147-1155 (2024) .

HL 39.10 Thu 12:00 POT/0081

Accurate electronic, optical, and magnetic properties of CrSBr via a tuned hybrid functional — •Daniel Hernangómez-Pérez[1], María Camarasa-Gómez[2], Javier Junquera[3], and Ashwin Ramasubramaniam[4] — [1]CIC nanoGUNE BRTA, Donostia, Spain — [2]Centro de Física de Materiales (CFM/MPC), Donostia, Spain — [3]Universidad de Cantabria, Santander, Spain — [4]University of Massachusetts Amherst, USA

CrSBr, a layered antiferromagnet, has attracted attention for its ambient stability, relatively high Néel temperature, and strong exciton-magnon coupling. While experiments have progressed rapidly, computational studies lag due to the high cost of many-body perturbation theory (MBPT). Here, we present a generalized Kohn-Sham density functional approach that accurately reproduces electronic bandstructures, optical spectra, exciton binding energies, and magnon spectra of bulk and few-layer CrSBr at much lower cost than MBPT. Using a minimal two-parameter set tuned to a few benchmarks, we achieve excellent agreement across a broad range of optoelectronic and magnetic properties.

M. Camarasa-Gómez, D. Hernangómez-Pérez, J. Junquera, A. Ramasubramanian (in preparation)

HL 39.11 Thu 12:15 POT/0081

Tunable exchange interaction and hysteresis observed via excitons in a van der Waals antiferromagnet bilayer — •Priyanka Mondal[1], Sonu Verma[2], Wenze Lan[1], Lukas Krelle[1], Ryan Tan[1], Regine von Klitzing[1], Kseniia Mosina[3], Zdenek Sofer[3], Akashdeep Kamra[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Department of Physics and Research Center OPTIMAS, Rheinland-Pf\"alzische Technische Universit\"at Kaiserslautern-Landau,Germany — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic

Two-dimensional magnets have emerged as key platforms for exploring layer-dependent magnetic phenomena. CrSBr is a recently identified van der Waals magnet with strong excitonic features and layered antiferromagnetic (AFM) order. While pristine bilayers show no magnetic hysteresis, we find that a ~3° twist induces clear hysteresis and can even stabilize a zero-field ferromagnetic state[1]. Field-dependent photoluminescence tracks this behavior through hysteretic exciton energy shifts that match the magnetic configuration. A two-sublattice model explains the response via twist-reduced interlayer exchange, allowing both parallel and antiparallel spin states. The bilayer behaves as an effective monodomain, switching cleanly into the AFM state without forming spin textures. These results highlight twist engineering as a route to programmable magnetic memory in 2D magnets.

[1] P. Mondal et al. arXiv preprint arXiv:2510.08018 (2025).