HL 40: 2D Materials and Heterostructures: Magnetic Properties

Time: Thursday 9:30–13:00 Location: EW 201

HL 40.1 Thu 9:30 EW 201

Optical properties of quasi-one-dimensional materials — •Thorsten Deilmann — Institute of Solid State Theory, University of Münster, Germany

Many of the atomically thin materials used today, such as graphene or MoS_2, exhibit a high in-plane symmetry. Anisotropic crystals unite the fascinating characteristics of the confined in-plane physics with their reduced crystal symmetry. This paves the way for polarization-sensitive applications, such as optical logic circuits operating in the infrared spectral region.

Here, we investigate and compare the doping-dependent optical properties of three different classes of materials from a first-principles perspective. Besides the well-known black phosphorus and the transition metal dichalcogenides ReS_2 and $ReSe_2$, we study the in-plane ferromagnetic CrSBr. Although all materials have a distinct anisotropy, the influence on the optical properties is intimately linked to the nature of the electronic quantum states.

HL 40.2 Thu 9:45 EW 201

Magnetic anisotropy in excitonic resonances and exciton-phonon coupling of the 2D magnetic semiconductor CrSBr — •Pierre-Maurice Piel[1], Nicolai-Leonid Bathen[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 material CrSBr comprises several intriguing characteristics: it is an optically active semiconductor and an air-stable 2D magnet with ferromagnetic ordering within each layer and antiferromagnetic coupling between adjacent layers. It has also a highly anisotropic electronic band structure, rendering it a quasi-one-dimensional electronic system [1]. In order to unravel the impact of magnetic order and magnetization direction on various aspects, including excitonic interband transitions, exciton-phonon coupling, and collective excitations, we employ magnetic field-dependent photoluminescence and resonant Raman experiments at low temperatures, around 4 Kelvin, well below the Néel temperature. We observe distinct differences for anti-ferromagnetic and ferromagnetic order in in the excitonic signatures from PL measurements and in resonant Raman spectra, both showing magnetic anisotropy for different crystallographic orientations. While the Raman-allowed first order phonon modes are unaffected by magnetization direction, new and well resolved magnetic-field dependent modes occur in the resonant-Raman spectra indicating strong exciton-phonon coupling. [1] J. Klein et al. ACS Nano, 17, 5316-5328 (2023)

HL 40.3 Thu 10:00 EW 201

Proximity effects in the valley Zeeman physics of van der Waals heterostructures — •Paulo E. Faria Junior and Jaroslav Fabian — University of Regensburg

Proximity effects are a hallmark of van der Waals systems, providing a very efficient way to functionalize the different materials in the heterostructure. Interestingly, these proximity effects arise from the small overlap of electron densities within the van der Waals gap. In this talk, I will address how proximity effects can be observed using the valley Zeeman physics of excitons in van der Waals heterostructures. Specifically, I will focus on three different scenarios: (i) the impact of electric field and interlayer distance fluctuations to interlayer exciton g-factors in MoSe2/WSe2 heterostructures[1]; (ii) the unexpected proximity-enhanced valley Zeeman shift in WS2/graphene systems[2]; and (iii) the emergence of an asymmetric valley Zeeman shift in MoSe2/CrSBr structures[3]. [1] Faria Junior, Fabian, Nanomaterials 13, 1187 (2023). [2] Faria Junior et al., 2D Mater. 10, 03400 (2023). [3] Serati de Brito, Faria Junior et al., arXiv:2309.03766, to appear in Nano Letters (2023). Funding: DFG SFB 1277.

HL 40.4 Thu 10:15 EW 201

Computational design of two-dimensional cold metal lateral heterojunction (Nb/Hf)Si_2N_4 tunnel diodes — •Paul Bodewei, Ersoy Sasioglu, Nicki Frank Hinsche, and Ingrid Mertig — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle (Saale), Germany

Cold metals have recently gained attention as a promising platform for innovative devices, such as tunnel diodes with negative differential resistance (NDR) [1] and field-effect transistors with subthreshold swings below the thermionic limit. Recently discovered two-dimensional (2D) transition metal carbides and nitrides have both metallic and semiconducting properties, making them ideal for these applications. We present a computational study of a prototype $NbSi_2N_4/HfSi_2N_4/NbSi_2N_4$ lateral heterojunction tunnel diode. Using density functional theory and a nonequilibrium Green function method, we investigate the current-voltage characteristics of these diodes with varying barrier thicknesses in zigzag and armchair orientations. Our results indicate negative differential resistance that leads to unconventionally high peak-to-valley current ratio (PVCR). Moreover, significant differences in peak current densities as well as PVCR for both armchair- and zigzag-orientations of the tunnel diodes have been found. These findings suggest that cold metal based materials hold promise for high PVCR NDR tunnel diodes, with potential applications in memory, logic circuits, and electronic devices. [1] Ersoy Şaşıoğlu and Ingrid Mertig, ACS Appl. Nano Mater. 6, 3758-3766 (2023).

HL 40.5 Thu 10:30 EW 201

Optical signatures of the magnetic order in CrSBr — •Marie-Christin Heissenbüttel[1], Pierre-Maurice Piel[2], Julian Klein[3], Thorsten Deilmann[1], Ursula Wurstbauer[2], and Michael Rohlfing[1] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]Physical Institute, University of Münster, Germany — [3]Department of Materials Science and Engineering, MIT, Massachusetts, USA

Controlling excitons in van der Waals coupled systems is a key idea to reveal tailored properties for the development of opto-electronic devices. Exciton energy and character in antiferromagnetic multilayer CrSBr can be controlled by an external magnetic field switching the internal magnetization to a ferromagnetic order. This modifies the optical response and we observe in our ab-initio GW/BSE calculations a distinct redshift, in accordance with corresponding measurements. We set up a minimal model to explain and convey the underlying physical mechanisms. Depending on the external field the coupling of adjacent layers is changed, shifting electronic states linearly in energy and excitons quadratically with respect to the field strength. While our results are generally valid for antiferromagnetic layered magnets, we uncover that the lowest excitation in CrSBr is optically dark and its detuning can also be controlled by the magnetic field.

HL 40.6 Thu 10:45 EW 201

Spectral-imaging of 2D magnetic semiconductor V-WS2 using ToF-XPEEM — •Q. Nguyen[1], O. Tkach[2,3], O. Fedchenko[2], S. Chernov[4], Z. Zhang[5], L. Hoang[5], M. Prandolini[4], D. Kutnyakhov[4], F. Pressacco[4], J. Dilling[4,7], L. Bruckmeier[4,7], M. Scholz[4], F. Scholz[4], C. Schlueter[4], K. Rossnagel[4,7], M. Kling[1,5], M. Hoesch[4], E. Pop[5], A. Mannix[5], T. Gorkhover[4,8], M. Dunne[1,5], N. Sirica[6], R. Schoenlein[1], H.-J. Elmers[2], and G. Schoenhense[2] — [1]SLAC Nat. Accel. Lab., USA — [2]Univ. Mainz — [3]SumDU, Ukraine — [4]DESY — [5]Stanford Univ., USA — [6]Los Ala. Nat. Lab., USA — [7]CAU Kiel — [8]Univ. Hamburg

Using x-ray element-selective, time-of-flight photoemission electron microscopy (ToF-XPEEM), we characterize the spatial distribution and spectroscopic signatures of p-type vanadium dopant within the 2D semiconductor WS2 - achieving unprecedented 1.0-micron spatial resolution. Multilayer WS2 islands ranging from 3 - 20-micron in lateral size are grown via hybrid metal-organic chemical vapor deposition with nominal vanadium dopant concentrations ranging from 4 to 30 atom%. Combined with the soft x-ray energies at PETRA III - P04, ToF-XPEEM measurements reveal unique elemental spectroscopic signatures that reflect the stoichiometry within each island - which is important for optimizing the growth of these semiconductors. The spatial maps unravel the atomic positions of vanadium and tungsten within the 2D flakes at different doping concentration. Complementary full-field, hard x-ray photoelectron diffraction measured at PETRA III - P22 and Bloch wave calculations reveal the structural properties.

15 min. break

Invited Talk HL 40.7 Thu 11:15 EW 201

Exciton transport in van der Waals antiferromagnet CrSBr
— •Florian Dirnberger[1], Sophia Terres[1], Akashdeep Kamra[2], Mikhail M. Glazov[3], and Alexey Chernikov[1] — [1]Institute of Applied Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Germany — [2]Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Saint Petersburg, Russia

The recent discovery of magnetic excitons - a rare type of optical excitation that emerges from spin-polarized electronic states in magnetic materials - raises important questions about elemental interactions between excitons, magnons, and light. Particularly the prototypical layered antiferromagnetic semiconductor CrSBr and its strongly bound excitons with large oscillator strength offer exceptional opportunities in this regard. In this talk, I will present the results of our study of the spatial transport of excitons in CrSBr with particular focus on the specific role of crystal anisotropy, magnons and magnetic order. Our experiments demonstrate highly non-linear exciton transport with unusual temperature dependence that culminates in substantially enhanced exciton propagation at the antiferromagnet-to-paramagnet phase transition. Observations of anomalous and effectively negative transport further highlight the profound coupling of excitonic, vibronic, and magnetic degrees of freedom in CrSBr.

HL 40.8 Thu 11:45 EW 201

Optoelectronic investigation of Berry curvature dipole induced non-linear anomalous thermal Hall effect in type-II Weyl Semimetal WTe_2 — •Ernst Knöckl[1,2] and Christoph Kastl[1,2] — [1]Walter Schottky Institut, Munich, Germany — [2]TU Munich, Germany

The Berry curvature forms the foundation for the topological classification of band structures. Importantly, it also impacts a material's (opto-)electronic properties, for example by introducing an anomalous transversal correction to the group velocity of charge carriers. Generally, symmetry constraints often preclude the observation of such effects, and only few, low-symmetry materials directly show relevant topological transport properties. In particular, few-layer WTe_2 has been shown to exhibit a nonlinear anomalous Hall effect [1] due to its low crystal symmetry and its strong Berry curvature dipole (BCD). We discuss the requirements for optically detecting a so far elusive thermal analogue of this effect, which is the socalled nonlinear anomalous thermal Hall effect (NLATHE). In principle, the NLATHE allows for experimentally accessing the first derivative of the BCD with respect to the chemical potential [2]. We present first results obtained on few-layer WTe_2 integrated into on-chip thermal circuits made from silicon nitride membranes.

[1] Sodemann, I., *et al.* Physical Review Letters 115.21 (2015): 216806
[2] Zeng, C., *et al.* Physical Review Research 2.3 (2020): 032066

HL 40.9 Thu 12:00 EW 201

Proximity Spin Physics in Twisted van der Waals Heterostructures — •Klaus Zollner[1], Paulo E. Faria-Junior[1], Simão M. João[2], Branislav K. Nikolić[3], and Jaroslav Fabian[1] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]Imperial College London, London SW7 2AZ, United Kingdom — [3]University of Delaware, Newark, DE 19716, USA

A crucial degree of freedom, to tailor proximity-induced spin interactions in van der Waals heterostructures, is the relative twist angle between the monolayers. We present comprehensive DFT-based results on twist- and gate-tunable proximity spin-orbit and exchange coupling in various 2D material heterostructures. Remarkably, in graphene/$Cr_2Ge_2Te_6$, the proximity exchange splitting of Dirac states can be reversed upon twisting, from 4 to −4 meV, while keeping the magnetization of $Cr_2Ge_2Te_6$ fixed [1]. In WSe_2/CrI_3, the valley splitting shows a gigantic tunability, from 0 to 12 meV (≈ 60 Tesla), combining twisting and gating [2]. In graphene/transition-metal-dichalcogenide bilayers, the spin-orbit coupling of proximitized Dirac bands can be tailored by several means [3]. Finally, we demonstrate the emergence of purely radial spin-orbit fields in twisted multilayers. We also relate our findings to experimentally verifiable fingerprints of proximity-induced spin interactions.

We acknowledge funding through DFG SFB 1277, DFG SPP 2244, and EU Horizon 2020 Program (Graphene Flagship).

[1] K. Zollner et al., PRL 128, 106401 (2022). [2] K. Zollner et al., PRB 107, 035112 (2023). [3] K. Zollner et al., arXiv:2310.17907 (2023).

HL 40.10 Thu 12:15 EW 201

Impact of proximity exchange coupled CrI_3 on WSe_2 valley dynamics — •Marc Schütte[1], Jo Bertram[1], Frank Volmer[2], Kenji Watanabe[3], Takashi Taniguchi[4], Christoph Stampfer[1], Lutz Waldecker[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics A and JARA-FIT, RWTH Aachen University, Aachen, Germany — [2]AMO GmbH, Advanced Microelectronic Center Aachen (AMICA), Aachen, Germany — [3]Research Center for Functional Materials, NIMS, Tsukuba, Japan — [4]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan

The optical selection rules of the transition metal dichalcogenides allow to individually address and manipulate their two energetically degenerate, but distinct, valleys in k-space. Lifting the degeneracy of the valley degree of freedom is possible via magnetic proximity coupling of adjacent layered magnetic materials. Here, thin layers of the two-dimensional layer-antiferromagnet CrI_3 are put into direct contact with monolayer WSe_2.
We present our findings about the valley dynamics in electrostatically gated, proximity exchange coupled CrI_3/WSe_2 heterostructures by optical reflection spectroscopy and time-resolved Kerr measurements. In particular, we find a type-II band alignment. This leads to charge separation within the heterostructure and long-lived valley polarizations within the WSe_2 valence bands. Excited polarizations furthermore show helicity dependent lifetime differences at particular gate voltages, which emerge from the modified band structure at K and K′.

HL 40.11 Thu 12:30 EW 201

Magnetic Field Dependent Raman Scattering in 2D Materials and Thin Films — •Hans Tornatzy, Manfred Ramsteiner, Joao Marcelo J. Lopes, and Markus R. Wagner — Paul-Drude-Institut, Berlin

Raman scattering by optical phonons in nonmagnetic materials is usually not considered to be magnetic field dependent. Despite this fact, a strong impact of magnetic fields on the intensity and polarization of Raman scattered light has recently been reported for the transition metal dichalcogenide (TMDC) MoS_2.[1,2] However, the underlying mechanisms of the oberserved phenomena are presently still a matter of debate. We present results on Raman scattering on related 2D materials as well as other thin films for which similarly remarkable influence of external magnetic fields is revealed. Our studies include also heterostructures containing 2D ferromagnetic materials such as $Fe_{3-5}GeTe_2$ which exhibits above room-temperature ferromagnetism and a perpendicular magnetic anisotropy (PMA). For the such hybrid systems, our results enable a facile way to probe the local magnetic field at the proximity of magnet/nonmagnet interfaces.

[1] Ji et al., PNAS 2016, 113, 9, p. 2349.
[2] Wan et al., RCS Adv. 2021, 11, p. 4035.

HL 40.12 Thu 12:45 EW 201

Electrical Observation of Skyrmions in the Sandwich Structure Incorporating Intrinsic Ferromagnetic Topological Insulators — •Takuya Takashiro[1], Ryota Akiyama[1], Ivan Kibirev[2], Andrey Matetskiy[2], Ryosuke Nakanishi[1], Shunsuke Sato[1], Takuro Fukasawa[3], Taisuke Sasaki[4], Haruko Toyama[1], Kota Hiwatari[1], Andrey Zotov[2], Alexander Saranin[2], Toru Hirahara[3], and Shuji Hasegawa[1] — [1]Department of Physics, The University of Tokyo, Tokyo, Japan — [2]Vladivostok, Russia — [3]Department of Physics, Tokyo Institute of Technology, Tokyo, Japan — [4]National Institute for Materials Science, Tsukuba, Japan

A topological insulator (TI) with ferromagnetism exhibits an energy gap at the Dirac point of the topological surface state (TSS), which provides a stage for interesting phenomena such as the quantum anomalous Hall effect and magnetic vortices, skyrmions. In particular, an intrinsic ferromagnetic TI, $Mn(Bi,Sb)_2Te_4$, has been actively studied because of a regularly arranged Mn-monolayer which induces ferromagnetism hybridizing with the TSS. In this study, we electrically observed skyrmions emerging in $Mn(Bi,Sb)_2Te_4$ layers in a sandwich structure of $Mn(Bi,Sb)_2Te_4/(Bi,Sb)_2Te_3/Mn(Bi,Sb)_2Te_4$ and found that skyrmions were stabilized by TSSs by tuning the Fermi level and the $(Bi,Sb)_2Te_3$-thickness. Intriguingly, the highly-ordered Mn monolayers make the skyrmions "soft-magnetic", which is promising for such as rewritable skyrmion memory (T. Takashiro, et al. Nano Lett. 22, 881 (2022)).