DS 2: 2D Materials and their Heterostructures I: hBN, WSe2, MoS2

Time: Monday 9:30–12:15 Location: A 060

DS 2.1 Mon 9:30 A 060

Strain activation of negatively charged boron vacancies in hexagonal boron nitride — •Xuankai Zhou[1], Jianpei Geng[2], Ruoming Peng[1], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, University of Stuttgart, Pfaffenwaldring 57, 70569, Stuttgart, Germany — [2]School of Physics, Hefei University of Technology, Hefei 230009, China

Spin defects in 2-dimensional materials have been extensively investigated since they offer a new playground for novel quantum phenomena, with improved scalability in device fabrication and the ability to study field and strain modulation. Negatively charged boron vacancy in hexagonal boron nitride (hBN) has been identified as an optically activated spin defect, hosting spin-1 ground states for quantum sensing. However, the emitted light from implanted boron vacancies tends to be dim, limiting their sensitivity. In this study, we made an important observation that the brightness of V_B^- is substantially enhanced when these vacancies are situated within the wrinkles and dislocations of hBN. Specifically, for hBN with a thickness of approximately 10 nm, we observed a remarkable increase of more than an order of magnitude in emission brightness, combined with an improved Optically Detected Magnetic Resonance (ODMR) contrast. Our findings shed light on the modulation of excited-state symmetry and the dynamics of underlying intermediate states in hBN induced by local strain and structure dislocation.

DS 2.2 Mon 9:45 A 060

Defect creation in hexagonal boron nitride by plasma treatment — •David Plitt, Felix Schaumburg, Timo Wagner, Martin Geller, Günther Prinz, Nicolas Wöhrl, and Axel Lorke — Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany

Hexagonal boron nitride (hBN) gained great attention after it was experimentally proven that their color centers exhibit single photon emission properties[1]. Simulations suggest that the emission wavelength of these color centers range from IR to UV[2], which was confirmed in experiments too[3]. Our measurements show that it is possible to create different color centers in the hBN structure using plasma treatment. This was achieved using different gases (argon, nitrogen and oxygen) and plasma parameters, including pressure, excitation power and distance to the plasma. The resulting color centers were then analyzed with photoluminescence measurements. Different excitation laser wavelengths were used and the measurements were conducted at room temperature as well as at low tempeatures. The produced defects cover the spectral range between 400 nm and 750 nm. A portion of the color centers exhibit time dependent optical properties like blinking and a shift in the emission wavelength.

[1] Zai-Quan Xu et. al., Nanoscale, 2018, 10, 7957 [2] Mehdi Abdi et. al., ACS Photonics 2018, 5, 1967-1976 [3] Suk Hyun Kim et. al., Nanomaterials 2023, 13, 2344

DS 2.3 Mon 10:00 A 060

Exciton-exciton interactions in heterobilayers of transition-metal dichalcogenides — •Edith Wietek[1], Alexander Steinhoff[2], Matthias Florian[3], Tommy Schulz[2], Takashi Taniguchi[4], Kenji Watanabe[4], Shen Zhao[5], Alexander Högele[5], Frank Jahnke[2], and Alexey Chernikov[1] — [1]Technische Universität Dresden, Deutschland — [2]Universität Bremen, Deutschland — [3]University of Michigan, USA — [4]NIMS, Ibaraki, Japan — [5]LMU München, Deutschland

Vertically stacked heterostructures of transition metal dichalcogenides (TMDCs) offer a versatile platform to study electronic and excitonic many-body effects. In particular, interactions between interlayer excitons are key to understand both non-linear optical and transport phenomena in these systems. Here, we address this topic in a joint experiment-theory study by considering spectrally narrow interlayer excitons in the moiré free limit of atomically reconstructed, hBN-encapsulated MoSe2/WSe2 heterobilayers. While classical dipolar repulsion is broadly assumed to determine exciton-exciton scattering, we demonstrate a major role of additional many-body effects including exchange interaction and dynamic screening. Identified by theory, these contribution compensate dipolar term, accounting for the observed spectral shifts of the interlayer excitons of only a few meV even for high injection densities close to the Mott transition threshold. Our findings challenge the traditional picture of the dipolar repulsion in van der Waals heterostructures, highlighting the major role of exchange and screening for the exciton-exciton interactions.

DS 2.4 Mon 10:15 A 060

Dielectric Function and exciton dynamics of 2-dimensional MoS_2 — •Lucas Krätschmer[1], Younes Slimi[1], Lukas Trefflich[2], Theo Pflug[3], Markus Olbrich[3], Noah Stiehm[1], Bernd Hähnlein[1], Sebastian Thiele[1], Chris Sturm[2], Alexander Horn[3], Marius Grundmann[2], Stefan Krischok[1], and Rüdiger Schmidt-Grund[1] — [1]Technische Universität Ilmenau, Ilmenau, Deutschland — [2]Universität Leipzig, Leipzig, Deutschland — [3]Hochschule Mittweida, Mittweida, Deutschland

2-dimensional MoS_2 belongs to the Transition Metal Dichalcogenide (TMD) family with a band gap of 1.7 eV, and thus has unique properties for optoelectronic applications. We present the dielectric function of a homogeneous MoS_2 film deposited on a sapphire substrate with a size of 1cm x 1cm in the spectral range of 0.5 to 6.5 eV. The sample was purchased commercially from the company Ossila B.V.. The static optical properties of the sample were determined by spectroscopic ellipsometry (SE), spatially integrated as well as spatially resolved to survey the local optical properties of the sample. We found that the integrated as well as the local optical response is quite similar, showing high homogenity of the film. We found further indications for grain boundaries (grain size approx. 1 μm) from the Ψ- and Δ-Maps. Based on these results, time-resolved imaging ellipsometry measurements are planned to investigate the dynamics of the exciton propagation.

DS 2.5 Mon 10:30 A 060

Photo-induced charge and spin transfer in the heterostructure CrSBr/$MoSe_2$ — •Andreas Beer[1], C. Serati de Brito[1,2], K. Zollner[1], P. E. Feria Junior[1], J. Fabian[1], H. S. J. van der Zant[3], Y. Galvao Gobato[2], and C. Schüller[1] — [1]University of Regensburg — [2]Universida de Federal de Sao Carlos — [3]Delft University of Technology

Van der Waals (vdW) heterostructures composed of two-dimensional (2D) transition metal dichalcogenides (TMDC) and vdW magnetic materials offer an intriguing platform to functionalize valley and excitonic properties in non-magnetic TMDCs. Here, we report a two color pump probe investigation of monolayer (ML) $MoSe_2$ on the layered A-type antiferromagnetic (AFM) semiconductor CrSBr. The material combination is predicted to feature a type III band alignment (broken bandgap), which leads to an p-doping in $MoSe_2$. This can already be suspected by photoluminescence, white light mapping and magneto-PL measurements, but can ultimately be shown by a pump probe technique. An ultrafast pump pulse creates free electrons in CrSBr. They can tunnel to $MoSe_2$ and reduce the background doping. The reduction can then be detected by an enhancement (reduction) in reflectivity of the $MoSe_2$ exciton (Trion). Remarkably by pumping the heterostructure with circular polarized light we can observe a long-lasting Kerr effect in the heterostructure. We explain our results by an out of plane spin component in the first layer of CrSBr.

15 min. break

DS 2.6 Mon 11:00 A 060

Photo-electrochemical thinning of transition metal dichalcogenides — •Simon Wörle[1], Jeremy Robinson[2], Franz Gröbmeyer[3], Emiliano Cortes[3], and Ian Sharp[1] — [1]Technical University of Munich — [2]Naval Research Laboratory, Washington, D.C — [3]Ludwig-Maximilians-Universität München

Two-dimensional transition metal dichalcogenides have attracted considerable attention due to their unique optoelectronic, mechanical and catalytic capabilities. For the application of 2D materials in semiconductor devices, the precise control of their properties is crucial, with the layer number being the most fundamental. Here, we demonstrate a top-down approach in aqueous solutions and under illumination to thin MoS_2, WS_2, $MoSe_2$ and WSe_2 layers of various thicknesses down to, in some cases, a self-limiting number of layers. The removal of the upper layers is initiated by laser illumination with wavelengths of 532nm and 785nm. In contrast to laser degradation in air, where

the TMD layers heat and sublimate, the thinning procedure in water is electrochemically driven. Photo-excited holes oxidize the surface layers in a self-limiting mechanism. An additional external voltage applied against a defined reference potential allows this thinning process to be further enhanced or prevented. For potentials larger than 0.8V vs Ag/AgCl, the thinning of MoS_2 occurs even under white light microscope illumination. The oxidation, starting at the edges or defects and spreading through the whole TMD flakes, can be in-situ monitored. The presented results show an overview of photo-electrochemical thinning of different TMDs under various bias and excitation conditions.

DS 2.7 Mon 11:15 A 060

DFT-assisted Investigation of Defects in 2D WSe2 by High-Resolution STEM and Differential Phase Contrast Imaging — •Maja Groll, Julius Bürger, Ioannis Caltzidis, Klaus D. Jöns, Wolf Gero Schmidt, Uwe Gerstmann, and Jörg K. N. Lindner — Department of Physics, Paderborn University, Germany

2D transition metal dichalcogenides and defects therein are currently the subject of intensive research due to their extraordinary optoelectronic properties. In particular, defects in monolayers, typically of vacancy type, are attracting much attention. Most spectroscopic investigations of material properties caused by defects are limited by the spatial resolution far above the atomic level. However, knowledge of the atomic structure is crucial for a detailed understanding of these properties. Modern scanning transmission electron microscopy (STEM) in combination with differential phase contrast imaging (DPC) allows for a structural analysis combined with the investigation of the electric field distribution at sub-atomic resolution. This enables the identification of defects and the resulting change in the field distribution. However, interpretation of STEM data is demanding because single substitutional atoms, such as oxygen, are difficult to detect and can nevertheless influence the physical and chemical properties. Here, vacancies in mechanically exfoliated 2D WSe2 flakes are analysed with focus on possible substitutional atoms. Conventional STEM at an acceleration voltage of 80keV in combination with STEM-DPC and density functional theory (DFT) calculations are used to characterize point defects and investigate their charge density distribution.

DS 2.8 Mon 11:30 A 060

Light-Matter coupling in Van der Waals heterostructures — •Bharti Parashar, Mathias Federolf, Atanu Patra, Vishakha Kaushik, and Sven Höfling — Technische Physik, University of Würzburg, Am Hubland 97074 Würzburg Germany

Transition metal dichalcogenides (TMDCs) heterostructures (HSs) offer a dynamic platform where artificially stacked monolayers of different TMDCs materials may reveal intriguing quantum behaviors. The alignment or twist between these monolayers generates a periodic moiré pattern, endowing the presence of the quasi-particle intralayer exciton, within the same material and an interlayer exciton characterized by charge carriers originating from different monolayers. Moiré superlattices in two-dimensional (2D) HSs induce quantum phenomena by fundamentally altering the electronic hybridizations by controlling the twist angle between atomically thin layers. This paradigm shift provides a unique avenue for precisely tailoring interactions between quantum particles and their coupling to electromagnetic fields. Moreover, beyond their discernible effects on single-particle states, strong moiré superlattices manifest excited states, such as the formation of moiré minibands of excitons [1]. In this study, we comprehensively explore the optoelectronic characteristics of twisted WSe2/WS2 van der Waals HSs. The insights obtained contribute to establishing a foundational understanding essential for realizing many-body states in moiré superlattices, such as exciton condensates, and bosonic insulating states via electric field manipulation.

Ref: [1] Jin, Chenhao, et al. Nature 567.7746 (2019): 76-80

DS 2.9 Mon 11:45 A 060

Large-area epitaxial growth and investigation of $Fe_{5-x}GeTe_2/WSe_2$ van der Waals heterostructures — •Hua Lv[1], Michael Hanke[1], Jens Herfort[1], Achim Trampert[1], Roman Engel-Herbert[1], Chen Chen[2], Joan Redwing[2], Manfred Ramsteiner[1], and J Marcelo Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, Pennsylvania, United States

Van der Waals heterostructures (vdWH) consisting of two-dimensional ferromagnets and transition metal dichalcogenides have attracted great interests due to their promising (opto)spintronic applications. The $Fe_{5-x}GeTe_2$ (FGT, with x $\sim$ 0.2) is considered as one of the most promising materials due to its high-temperature ferromagnetic order and robust perpendicular magnetic anisotropy (PMA). We report on the large-area MBE growth of FGT on CVD-grown $WSe_2/Al_2O_3(0001)$. The structural characterizations reveal the high-quality formation of FGT/WSe_2 vdWH. The anomalous Hall effect (AHE) exhibits a clear hysteresis loop below 250 K providing evidence for PMA. The S-shaped AHE at higher temperatures indicates a magnetic order up to 360 K. Further magnetotransport anomaly can be explained by the formation of skyrmions accompanied by a topological Hall effect and a non-colinear magnetic order contribution to the magnetoresistance. Our results demonstrate the extraordinary potential of high-quality FGT/WSe_2 vdWH for tailoring proximity-induced phenomena that can be exploited for (opto)spintronic applications.

DS 2.10 Mon 12:00 A 060

multi-strategy coordination enables WSe2 to achieve high-performance real-world detection of NO2 — •Yu Duan[1,2], Sam Zhang[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Center for Advanced Thin Films and Devices, School of Materials and Energy, Southwest University, Chongqing, 400715, China

In recent years, WSe2 has become an ideal material for room-temperature NO2 gas sensing, but its low response and long response time limit its application. In this study, we combined multiple strategies of constructing a three-dimensional structure, introducing Se vacancies, Au nanoparticle sensitization, and 1T/2H-phase modulation. The synergistic effect was utilized to effectively enhance the gas adsorption, charge transfer degree, and carrier transport capacity of WSe2 and achieve high-performance NO2 detection. The prepared V-WAAP achieved high response (78.32%) with a short response time (33 s), and outstanding stability and selectivity for low concentration (1 ppm) NO2. The intrinsic factors of sensing performance improvement were comprehensively analyzed by combining the results of compositional and structural characterization. In addition, we verified its potential for practical applications by assembling a V-WAAP-based NO2 gas sensing equipment.