HL 53: 2D Semiconductors and van der Waals Heterostructures V

The session covers excitonic properties of 2D semiconductors and van der Waals heterostructures.

Time: Thursday 15:00–17:15 Location: H15

HL 53.1 Thu 15:00 H15

1D exciton confinement in monolayer $MoSe_2$ near ferroelectric domain walls in periodically poled $LiNBo_3$ — •Pedro Soubelet, Yao Tong, Asier Astaburuaga Hernandez, Andreas V. Stier, and Jonathan J. Finley — Walter Schottky Institut and TUM School of Natural Sciences, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

Monolayer transition metal dichalcogenides are an emergent platform for exploring and engineering quantum phenomena in condensed matter. Due to their atomic thickness, the excitonic response is highly influenced by the dielectric environment. In this work, we explore the optical properties and exciton kinetics of monolayer thick $MoSe_2$ straddling domain wall boundaries in ferroelectric periodically poled $LiNbO_3$ (PPLN). Spatially resolved photoluminescence (PL) experiments reveal sorting of neutral and charged excitons across the boundary. Our results reveal evidence for extremely large in-plane electric fields ($\simeq$4000 kV/cm) at the domain wall (DW), whose effect is manifested in the routing of free charges and trions towards oppositely poled domains, resulting in a nonintuitive spatial PL intensity pattern. In a second step, we engineer the PPLN substrate and the 2D heterostructure to exploit the non-uniform in-plane electric field exerted by the DW to confine neutral excitons in a 1D dipolar gas. Reducing the dimensionality holds an excellent potential for unlocking strong exciton-exciton interaction regimes, enabling exploration of exotic quantum phases of matter and designing advanced optoelectronic devices.

HL 53.2 Thu 15:15 H15

Collective charge excitations between moiré minibands in twisted WSe_2 bilayers probed with resonant inelastic light scattering — •Hendrik Lambers[1], Nihit Saigal[1,2], Nicolai-Leonid Bathen[1], Veljko Antić[1], Lennart Klebl[3], Dante M. Kennes[4], Tim O. Wehling[3], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Germany — [2]EMBL Imaging Centre, Heidelberg, Germany — [3]Institute of Theoretical Physics, University of Hamburg, Germany — [4]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany

The weak van der Waals coupling between monolayers of transition-metal dichalcogenides (TMDCs) allows the realization of twisted van der Waals structures resulting in precisely tailored 2D quantum systems with superimposed moiré superlattice structures. These are dependent on twist angle and lattice constant mismatch and can cause flat moiré mini bands in the reduced Brillouin zone of the superlattice. Here we study these moiré minibands in $tWSe_2$ homobilayers encapsulated in hBN by low temperature resonant inelastic light scattering (RILS) [1]. Guided by theoretical predications, we identify single particle-like collective inter moiré miniband excitations. Thereby, we establish RILS as a tool to quantitatively probe the formation of moiré minibands. Furthermore, we identify local twist angle variations by lateral force microscopy and correlate these findings with optical (Raman) spectroscopy. [1] N. Saigal et al., Phys. Rev. Lett. 133, 046902 (2024).

HL 53.3 Thu 15:30 H15

Unraveling Rashba spin-orbit coupling in TMDs — •Miguel Morales Cocera[1,2], Marta Prada[1], and Gabriel Bester[1] — [1]University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

Transition metal dichalcogenides (TMDs) possess unique optical and electronic properties, making them ideal candidates for exploring new physical phenomena. Their significant spin-orbit coupling enables a rich landscape of spin-valley physics within the realm of excitonic effects or topologically non-trivial materials, to name a few. However, there are still unanswered questions concerning the mechanisms that rule Rashba spin-orbit coupling (RSOC), such as the role of the atomic and orbital composition, number of layers, or band character. In this work, we employ ab-initio calculations together with perturbative approaches to unravel the intricacies of bilayer TMDs with an intrinsic dipole, which is far from trivial. We deliver with high numerical precision the Rashba parameters in Rmx (Bernal stacking) bilayers (M=Mo, W. X=S, Se, Te).

HL 53.4 Thu 15:45 H15

Theory of Magnetic Field Dependence of Excitonic Spectra in Atomically Thin Semiconductors — •Michiel Snoeken and Henry Mittenzwey — Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Hardenbergstraße 36, 10623 Berlin, Germany

The linear absorption spectrum of TMDC monolayers under the influence of an in-plane magnetic field is theoretically studied in an excitonic picture. It is shown that in-plane magnetic fields induce a hybridization between spin-bright and spin-dark exciton transitions, resulting in a brightening of spin-dark excitons in the linear absorption spectrum with increasing in-plane field-strength. Numerical evaluation shows that with increasing field strength, not only the energy splitting between bright and dark excitonic resonances increases, but also an impact on the respective excitonic linewidths can be observed. Some limiting cases are investigated analytically, allowing to discuss a detailed physical picture of the magnetic field-dependent excitonic energies and linewidths.

15 min. break

HL 53.5 Thu 16:15 H15

Spatial mapping of the tunable band gaps of bilayer graphene using a WSe_2 sensor layer — David Tebbe[1], •Alexander Polkowski[1], Sophia Lackhoff[1], Jonas Blum[1], Takashi Taniguchi[2], Kenji Watanabe[2], Bernd Beschoten[1,3], Lutz Waldecker[1], and Christoph Stampfer[1,4] — [1]2nd Institute of Physics A, RWTH Aachen University, Aachen — [2]National Institute for Materials Science, Namiki, Tsukuba, Japan — [3]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany — [4]Peter Grünberg Institute (PGI-9) Forschungszentrum Jülich, Jülich, Germany

Bernal bilayer graphene (BLG) is a 2D material with promising properties for future quantum technologies, due to its tunable band gap and rich correlated phases, which have been detected by electrical transport measurements. However, due to their nature, these measurements have not been able to spatially resolve the bandgap and other electronic properties of BLG. Here, we show optical sensing can overcome this limitation. To achieve this we place a sensing monolayer of WSe_2 in direct contact to BLG in a double-gated device structure. The sensor layer hosts excitons, with the ability to sense changes in the electronic configuration of the BLG. The WSe_2 hosts Rydberg excitons, which are sensitive to the surrounding dielectric environment and thus sense small changes in carrier density within the BLG, allowing to observe the band gap opening. These excitonic states can be resolved using white light reflection spectroscopy, which allowed us to spatially map the potential landscape in the BLG.

HL 53.6 Thu 16:30 H15

Beyond the K-Valley: Exploring Unique Trion States in Indirect Band Gap Monolayer WSe_2 — •Franz Fischer[1,2], Carl Emil Mørch Nielsen[1], and Gabriel Bester[1] — [1]University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

Atomically thin layers of transition metal dichalcogenides are of great interest due to their exceptional electronic and optical properties. Their lack of inversion symmetry and strong spin-orbit interaction from heavy metal atoms leads to an additional valley degree of freedom and significant spin splittings in the Brillouin zone. The reduced dimensionality and dielectric screening make these materials ideal for studying Coulomb-bound many-body states, such as excitons and trions.

We will discuss calculations of the optical properties of monolayer WSe_2 using *ab initio* many-body screened configuration interaction. We'll highlight our findings on additional species of negatively charged trions including the **Q**-valley, which we found to be more energetically favorable than those in the **K**-valley. Our results align well with ex-

perimental data and provide new insights into previously observed but unexplained optical features. Furthermore, we will analyze the many-body interactions that reveal the mechanisms behind the increased singlet-triplet splitting and the redshifted energies in the **Q**-valley trions compared to those in the **K**-valley.

HL 53.7 Thu 16:45 H15

Trion saturation and trion filtering in MoS_2 and MoS_2/graphene heterostructures — Omid Ghaebi[1], Tarlan Hamzayev[1], •Till Weickhardt[1], and Giancarlo Soavi[1,2] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena — [2]Abbe Center of Photonics, Friedrich Schiller University Jena

Optical excitation of electron-hole pairs in transition-metal dichalcogenides leads to the formation of excitons, that can join with free carriers to form trions [1]. Since trions display an efficient non-radiative decay, tuning their relative density with respect to neutral excitons by external knobs is fundamental to engineer the light emitting efficiency of TMD opto-electronic devices. In this work, we investigate the interplay of excitons, trions, and free electrons with regards to gating and excitation power. By carrying out these experiments on a pristine MoS_2 monolayer as well as on a MoS_2/graphene heterostructure where the graphene facilitates fast charge transfer from the TMD [2,3], we study the interdependent dynamic of excitons and trions. Most prominently, this effect can be seen in a super-linear power-scaling of the exciton density due to saturation of trions in the monolayer MoS_2 [4]. When the graphene is added to form the heterostructure, this effect vanishes due to the elimination of trions.

[1] Mak et al. Nature Mater 12, 207-211 (2013). [2] Lorchat et al. Nat. Nanotechnol. 15, 283-288 (2020). [3] Küchle et al. Opt. Mater.: X 12, 2590-1478 (2021). [4] Wang et al. ACS Photonics 10 (2), 412-420 (2023).

HL 53.8 Thu 17:00 H15

Engineering carrier density and exciton polarization in WSe2 monolayers via photochlorination — •Eirini Katsipoulaki[1,2], George Vailakis[1,3], Delphine Lagarde[4], Vishwas Jindal[4], Konstantinos Mourtzidis[4], Xavier Marie[4], Ioannis Paradisanos[1], George Kopidakis[1,3], George Kioseoglou[1,3], and Emmanouel Stratakis[1,2] — [1]FORTH/IESL, Heraklion, Greece — [2]Dpt. of Physics, UoC, Heraklion, Greece — [3]Dpt. of Materials Science and Engineering, UoC, Heraklion, Greece — [4]Universite de Toulouze, INSA-CNRS-UPS, LPCNO, Toulouze, France

Transition Metal Dichalcogenides (TMDs) represent a special class of 2D van der Waals materials. Unlike their 3D-counterparts, which are indirect gap semiconductors, the monolayers exhibit a direct bandgap, leading to a significant enhancement in photoluminescence quantum yield. TMDs feature valley dependent optical selection rules, establishing them as promising candidates for atomically thin optoelectronic devices. A key factor influencing the performance of TMDs in these applications is the carrier density. To address this, we demonstrate the modulation of the Fermi level in WSe2 monolayers using an UV-assisted photochlorination method. Systematic shifts and relative intensities between charged and neutral excitons indicate a controllable decrease of the electron density and switch WSe2 from n- to a p-type semiconductor. DFT calculations predict Cl2 adsorption at Se vacancies. Furthermore, this method can strongly impact the circular polarization degree of excitons. These findings indicate that photochlorination can tailor nanopatterned lateral p-n junctions.