CPP 25: 2D Materials 6 (joint session DS/CPP)

Time: Wednesday 11:15–13:00 Location: H17

CPP 25.1 Wed 11:15 H17

Curvature-induced spin-orbit splitting in transition metal dichalcogenide nanotubes and wrinkles — Mohammadreza Daqiqshirazi and •Thomas Brumme — Theoretical Chemistry, TU Dresden

Strain engineering provides a powerful means to tune the properties of 2D materials. Homogeneous strain fields have been studied extensively, and there are standard techniques for altering properties of 2D materials even in industry. On the other hand, much less is known about how inhomogeneous strain affects the electronic properties of 2D materials. We employed DFT to understand the correlation between the atomic and the electronic structure in nanoscale wrinkles and nanotubes of the prototypical transition metal dichalcogenide WSe_2. Our research shows that the symmetry breaking in these structures lead to strong Rashba-like spin-orbit splitting of the bands at the Γ point and that they thus may be utilized in future tunable spintronics devices.

CPP 25.2 Wed 11:30 H17

Moiré-Bose-Hubbard model for interlayer excitons in twisted transition metal dichalcogenide heterostructures — •Niclas Götting, Frederik Lohof, and Christopher Gies — Institute for Theoretical Physics, University of Bremen, Bremen

Introducing a twist between two superimposed TMD monolayers results in a new superlattice whose properties heavily depend on the twist angle. These so-called moiré structures of TMD materials like MoS_2/WS_2 can host interlayer excitons (IXs) which perceive the varying atomic registry over the moiré unit cell as an effective moiré potential. In such structures, correlated states can emerge, in which the IXs are strongly localized to the potential minima due to exciton-exciton interactions.

We investigate the phases of these trapped moiré IXs by approximating them as bosonic particles and mapping the system onto a Bose-Hubbard model [1]. Our methods allow us to calculate the hopping and two-particle interaction terms of the Bose-Hubbard model for n-th nearest neighbors. To examine the strong impact of dielectrics surrounding the heterobilayer, we introduce a Keldysh potential to the calculation and thereby obtain first results of the twist-angle dependent phases of moiré IXs in twisted TMD heterobilayers.

[1] Götting et al., Phys. Rev. B 105, 165419 (2022)

CPP 25.3 Wed 11:45 H17

Enhanced Potassium Storage Capability of Two-Dimensional Transition-Metal Chalcogenides — •Vincent Hartmann and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Potassium-ion batteries (PIBs) have been considered a promising alternative to lithium-ion batteries due to their merits of high safety and low cost. Two-dimensional transition metal chalcogenides (2D TMCs) with high theoretical specific capacities and unique layered structures have been proven to be amenable materials for PIB anodes. However, some intrinsic properties including severe stacking and unsatisfactory conductivity restrict their electrochemical performance, especially rate capability. Herein, a heterostructure of high-crystallized ultrathin MoSe2 nanosheet-coated multiwall carbon nanotubes was prepared and its electrochemical properties were investigated. In such a heterostructure, the constructive contribution of CNTs not only suppresses the restacking of MoSe2 nanosheets but also accelerates electron transport. Meanwhile, the MoSe2 nanosheets loaded on CNTs exhibit an ultrathin feature, which can expose abundant active sites for the electrochemical reaction and shorten the K+ diffusion length. Therefore, the synergistic effect between ultrathin MoSe2 and CNTs endows the resulting nanocomposite with superior structural and electrochemical properties. Additionally, the high crystallinity of the MoSe2 nanosheets further leads to the improvement of electrochemical performance.

CPP 25.4 Wed 12:00 H17

Single photon emission of quantum emitters in WSe2 monolayers and their temperature-dependent coherence properties — •Martin von Helversen[1], Paul Schlaugat[1], Chirag Palekar[1], Carlos Antón-Solanas[2], Bárbara Rosa[1], Christian Schneider[2], and Stephan Reitzenstein[1] — [1]Institute for solid state physics, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institute for Physics, Carl von Ossietzky Universtität Oldenburg, 26111 Oldenburg, Germany

Two-dimensional van der Waals monolayers have appeared as novel type of semiconducting materials, which provide a platform for the exploration of their highly interesting optical, electronic and structural properties. Within the transition-metal dichalcogenides, WSe2 has turned out to be the most promising platform for two-level single-photon emitters, generated either by applied strain to the monolayer-flake [1,2], or by defects in the material [2]. However, the quality of the generated photons still lacks behind other systems as for example semiconductor quantum dots. In this work, we study single emitters of a strained WSe2-monolayer showing linewidths around 100 μeV at 4 K. In quasi-resonant pulsed optical excitation a second-order autocorrelation value down to $g^{(2)}(0)$=0.037(5) is measured. We further study their temperature dependent first-order coherence properties via a scanning Michelson interferometer, which yields coherence times up to 48 ps.

[1] L. N. Tripathi et al., ACS Photonics 5, 1919 (2018)
[2] K. Parto et al., Nat. Commun. 12, 3585 (2021)

CPP 25.5 Wed 12:15 H17

Spin-defect characteristics of single sulfur vacancies in monolayer MoS_2 — •Alexander Hötger[1], Tomer Amit[2], Julian Klein[3], Katja Barthelmi[1], Thomas Pelini[4], Alex Delhomme[4], Sergio Rey[5], Marek Potemski[4,6], Clément Faugeras[4], Galit Cohen[2], Daniel Hernangómez-Pérez[2], Takashi Taniguchi[7], Kenji Watanabe[7], Christoph Kastl[1], Jonathan Finley[1], Sivan Refaely-Abramson[2], Alexander Holleitner[1], and Andreas Stier[1] — [1]Walter Schottky Institute, Garching, Germany — [2]Weizmann Institute of Science, Rehovot, Israel — [3]Massachusetts Institute of Technology, Cambridge, USA — [4]Laboratoire National des Champs Magnetiques Intenses, Grenoble, France — [5]Technical University of Denmark, Lyngby, Denmark — [6]University of Warsaw, Warszawa, Poland — [7]National Institute for Materials Science, Tsukuba, Japan

Single spin defects in 2D transition-metal dichalcogenides are natural spin-photon interfaces for quantum applications. Here we report high-field magneto-spectroscopy from three emission lines of He-ion induced sulfur vacancies in monolayer MoS_2. The distinct valley-Zeeman splitting and the brightening of dark states necessitates spin-valley selectivity of the defect states and lifted spin-degeneracy at zero field. Comparing our results to ab-initio calculations identifies the nature of the defect luminescence. Analysis of the optical degree of circular polarization reveals that the Fermi level is a parameter that enables the tunability of the emitter. These results show that defects in 2D semiconductors may be utilized for quantum technologies.

CPP 25.6 Wed 12:30 H17

Probing excitonic population dynamics by nonlinear optical wave mixing in monolayer WSe2 — •Jonas M. Bauer, Lijue Chen, Philipp Wilhelm, Sebastian Bange, John M. Lupton, and Kai-Qiang Lin — Department of Physics, University of Regensburg, 93053 Regensburg, Germany

Monolayer semiconductors are emerging platforms for strong nonlinear light-matter interaction, due to their giant oscillator strength of tightly bound excitons. Recently, we reported the existence of a new excitonic species, the high-lying exciton (HX), in monolayer WSe2. The HX appears at around twice the energy of the band-edge A-exciton, forming a ladder-type excitonic three-level system. We demonstrate excitonic quantum interference in monolayers [1] and twisted bilayers [2]. Here, we apply time-resolved nonlinear spectroscopy to probe the excitonic dynamics. We find that a significant time difference between two light pulses is necessary for optimal sum-frequency generation (SFG) and four-wave mixing (FWM) if one of the pulses is in resonance with an excitonic transition. The experimental results are rationalized by numerical calculations based on a density-matrix approach and provide insights into coherent exciton dynamics on a femtosecond scale.

[1] K.-Q. Lin, S. Bange, & J. M. Lupton, Nat. Phys. 15, 242-246 (2019).
[2] K.-Q. Lin, J.M. Bauer et al., Nat. Commun. 12, 1553 (2021).

CPP 25.7 Wed 12:45 H17

Characterization of 2D WSe2 by high-resolution STEM and Differential Phase Contrast STEM — •Maja Groll[1], Julius Bürger[1], Ioannis Caltzidis[2], Marc Sartison[2], Klaus Jöns[2], and Jörg Lindner[1] — [1]Nanostructuring, Nanoanalysis and Photonic Materials Group, Department of Physics, Paderborn University, Germany — [2]Hybrid Quantum Photonic Devices, Department of Physics, Paderborn University, Germany

2D transition metal dichalcogenides (TMDs) are gaining attention as their optical and electronic properties differ from those of their bulk counterparts. In particular, layer thickness-dependent properties, such as the transition from an indirect to a direct band gap in monolayers, make these materials interesting for photonic and optoelectronic applications. At the same time 2D-TMDs are ideal materials for the advancement of new techniques in scanning transmission electron microscopy (STEM) like differential phase contrast (DPC)-STEM. Using a spherical aberration corrected STEM, this technique enables the quantification of atomic electric fields with sub-atomic resolution if the specimen is sufficiently thin. In order to examine the atomic electric fields of TMDs, we transferred mechanically exfoliated mono- and multilayers of tungsten diselenide (WSe2) to TEM grids. The atomic structure of WSe2 flakes and their thickness are studied using TEM, energy filtered TEM and STEM. STEM-DPC measurements are performed using an eight-fold segmented bright-field STEM detector measuring the beam deflection due to the internal fields. Results are presented for WSe2 flakes of different thickness and compared with simulations.