HL 49: Quantum Emitters in 2D Semiconductors

Time: Thursday 16:15–17:30 Location: POT/0081

Invited Talk HL 49.1 Thu 16:15 POT/0081

Phonon-mediated nonlinearity and defects in hexagonal boron nitride — •Nahid Talebi — Institute of Experimental and Applied Physics, Kiel University, Germany

Hexagonal boron nitride (hBN) hosts a rich phonon landscape whose strong oscillator strengths in the first and second Reststrahlen bands give rise to negative permittivity and support the propagation of hyperbolic phonon polaritons. In this work, we show that these phonon modes can mediate highly efficient down-conversion of optical excitation, enabling strong coupling to point defects and facilitating the coherent excitation of their electronic states. We further demonstrate that such defect states in hBN can couple efficiently to excitons in hybrid hBN*perovskite structures, establishing a robust exciton*defect interaction channel. Remarkably, we find that excitonic energy can be transported over distances up to 150 micrometers through incoherent hopping across a defect network within hBN. By combining spatially and spectrally resolved photoluminescence and cathodoluminescence spectroscopy, we identify the mechanisms governing coherent and incoherent defect excitation and reveal the interplay and strong coupling among excitons, defects, and phonons in hBN. These insights establish hBN as a versatile platform for phonon-assisted light*matter interactions and long-range energy transport in hybrid quantum nanophotonic systems.

HL 49.2 Thu 16:45 POT/0081

Spin Dynamics of Quantum Sensors Based on Hexagonal Boron Nitride — •Paul Konrad[1], Andreas Sperlich[1], Igor Aharonovich[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg — [2]School of Mathematics and Physical Sciences, University of Technology Sydney, Ultimo, NSW 2007, Australia

Colour centres in solid-state materials show great potential in quantum information technology and sensing applications. The spin triplet system of the lately discovered negatively charged boron vacancy ($V_B{}^-$) in hexagonal boron nitride (hBN) can be exploited in terms of its application as temperature, magnetic field, and pressure sensor.[1] Increasing the sensitivity of these nano-scale sensors is a crucial step towards application and requires not only controlled generation[2] but deep knowledge about the dynamics of the system. This includes predicted but experimentally hardly accessible intermediate states.

In this study, we achieve a direct measurement of a 24.0(3) ns relaxation time from the dark intermediate state to the ground state at room temperature, which approximately doubles at low temperatures. These findings are corroborated by detailed simulations of populations. Accounting for this relaxation considerably enhances spin manipulation efficiency, allowing substantial optimization of the quantum sensor's sensitivity based on boron vacancies.[3]

[1] Gottscholl et al., *Nat. Commun.*, **12**, 4480 (2021).
[2] Patra et al., *Adv. Funct. Mater.* e17851 (2025).
[3] Konrad et al., *arXiv* preprint arXiv:2503.22815 (2025).

HL 49.3 Thu 17:00 POT/0081

Exciton-enhanced light emission in pristine and doped MoS_2 from ab initio calculations — •Adriana Bocchini[1], Djennane Khaoula[2], Henry Hübschmann[1], Nikita Siverin[3], Andreas Farenbruch[3], Maja Groll[1], Klaus Jöns[1], Gerhard Berth[1], Dmitri Yakovlev[3], Wolf Gero Schmidt[1], and Uwe Gerstmann[1] — [1]Universität Paderborn, Germany — [2]Yahia Fares University of Medea, Algeria — [3]Technische Universität Dortmund, Germany

Two-dimensional transition metal dichalcogenides (2D-TMDs) are emerging as a suitable alternative in a variety of electronic and optoelectronic devices [1,2]. The properties of this family, in fact, can be systematically customized upon structural modification, e.g., via exfoliation or dopants. Notably, most of these properties are strongly determined by excitons, the formation of which is strongly facilitated by defects [3]. In this study, we use DFT routines to systematically investigate the influence of excitons on the optical properties of MoS_2 films. Thereby, we do not only analyze the dependency of the optical response on the layer thickness, but also their evolution upon the application of external electric fields or by twisting the layers relative to each other. In addition, we model MoS_2-based Janus structures by selectively substituting some of the S atoms with heavier chalcogens and analyze the suitability of these configurations as possible light-emitting solid-state quantum dots.

[1] R. Thayil,, *et al.*, Small **21**, 2412467 (2025)
[2] S. Joseph, *et al.*, Mater. Chem. Phys. **297**, 127332 (2023)
[3] J. Qu *et al.*, ACS Nano **18**, 34322 (2024)

HL 49.4 Thu 17:15 POT/0081

Thermodynamic properties of quantum defects in boron nitride using machine-learned force fields — •Ariel Moises Cabrera Aguilar and Carla Verdi — The University of Queensland, Brisbane, Australia

Hexagonal boron nitride (hBN) has emerged as an excellent host material for bright single-photon emitters. Experimental and computational studies associate these single-photon emitters (SPEs) in hBN predominantly with carbon-related defects. However, the lack of first-principles calculations at finite temperatures and with sufficiently large supercells hinders the establishment of a consensus on the most likely defect candidates for quantum-technology applications. Machine-learned force fields (MLFFs) provide highly accurate finite-temperature simulations because they can be trained to reproduce first-principles energies and forces across diverse configurations. We trained a MLFF capable of describing various carbon cluster defects (C_B, C_N, C_BC_N, C_BV_N, C_BC_i, and C_NC_i) at temperatures up to approximately 2000 K. To evaluate the accuracy of the force field in reproducing atomic positions, interatomic energies, and forces across these structures, we compute formation energies, phonon dispersions, and photoluminescence spectra, and compare these quantities with available experimental data. The force field successfully reproduces the line shape of several defects in multilayered systems of different supercell sizes. The MLFF is used to investigate multiple defects in large supercells over long molecular dynamics simulation times, allowing us to capture metastable structures that emerge at finite temperature.