

HL 26: 2D Materials and Heterostructures: Quantum Emitters and Defects

Time: Wednesday 9:30–12:15

Location: EW 201

HL 26.1 Wed 9:30 EW 201

Spin Dynamics of Quantum Sensors Based on Hexagonal Boron Nitride — ●PAUL KONRAD¹, ANDREAS SPERLICH¹, IGOR AHARONOVICH², and VLADIMIR DYAKONOV¹ — ¹Experimental Physics 6, Julius-Maximilians-University Würzburg, 97074 Würzburg — ²School 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 lately discovered negatively charged boron vacancy (V_B^-) in hexagonal boron nitride (hBN)^[1] has shown that the defect exhibits a spin-triplet ground state with spin-dependent photoluminescence. The system can be exploited in terms of its application as temperature, magnetic field, and pressure sensor [2,3] which extends the already known applications of e.g. NV-centers in diamond not only due to its 2D character but also by highly improved temperature sensing especially at low temperatures.

Here we present new insights into the spin dynamics of V_B^- in form of measurements of ground-state repopulation after pulsed laser excitation. For these studies we record transient photoluminescence with sub-nanosecond accuracy and determine the influence of the relaxation dynamics on the coherent control of the quantum system. This information can be used to optimize pulse timing.

- [1] Gottscholl et al., *Nat. Mat.*, **19**, 5, 540 (2020).
- [2] Gottscholl et al., *Sci. Adv.*, **7** (14), eabf3630 (2021).
- [3] Gottscholl et al., *Nat. Commun.*, **12**, 4480 (2021).

HL 26.2 Wed 9:45 EW 201

Dephasing Dynamics in Defect Centers of Hexagonal Boron Nitride Probed by Time-Resolved Cathodoluminescence Spectroscopy — ●NAHID TALEBI^{1,2}, MASOUD TALEB^{1,2}, PAUL BITTORF¹, MAXIMILIAN BLACK¹, MARIO HENTSCHEL³, and KOUROSH ESMAEELI KOSHKOIE³ — ¹Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — ²Birkenweg 20 — ³34th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany

Defect centers in hexagonal boron nitride (hBN) have been extensively explored as room-temperature single-photon sources. The electronic structures of these defects exhibit strong coupling to phonons, as evidenced by the observation of phonon sidebands in both photoluminescence and cathodoluminescence spectra, and as reported in the literature. However, the dynamics of the electron-phonon coupling as well as phonon-mediated dephasing of the color centers in hBN have remained unexplored. Here, we apply a novel time-resolved CL spectroscopy technique (Nature Physics 19, 869*876 (2023)) to explore the population decay to phonon states and the dephasing time T2 with sub-femtosecond time resolution. We demonstrate an ultrafast dephasing time of only 200 fs and a population decay of approximately 700 fs at room temperature, in contrast with all-optical time-resolved photoluminescence techniques that report a decay of a few nanoseconds. This behavior is attributed to an efficient excitation of coherent phonons polaritons in hBN with electron beams that results in faster dephasing of electronic transitions.

HL 26.3 Wed 10:00 EW 201

Radial quasi Bound States in the Continuum fabricated from Hexagonal Boron Nitride — ●CONNOR HEIMIG, JONAS BIECHTELER, THOMAS WEBER, LUCA SORTINO, and ANDREAS TITTL — Chair in Hybrid Nanosystems, Nanoinstitute Munich, Faculty of Physics, Ludwig-Maximilians-Universität München, 80539 Munich, Germany

We present a novel class of optical metasurfaces through the integration of the radial quasi Bound State in the Continuum (qBIC) concept into the realm of 2D van der Waals materials. Our design is underpinned by Radial qBICs, arising from structural asymmetry in a ring of trapezoid pair resonators fabricated from hexagonal Boron Nitride (hBN).

Overcoming the trade-off between refractive index and optical losses, symmetry-broken qBICs efficiently suppress radiation losses from hBN, enabling high-Q resonances across the entire visible spectrum. Leveraging the unique properties of a low-refractive index van der Waals material such as hBN, allows the development of a novel nanophotonic platform for enhanced light-matter interaction. This integrated

approach further establishes an experimental foundation for the implementation of hBN as a photonic medium for metaoptics, offering prospects for compact, spectrally selective, and polarization-invariant metadevices for diverse on-chip photonics applications.

HL 26.4 Wed 10:15 EW 201

Controlling the emission intensity of hBN emitters by graphene gates — ●CORINNE STEINER^{1,2}, REBECCA RAHMEL¹, FRANK VOLMER³, PATRICIA PESCH¹, KENJI WATANABE⁴, TAKASHI TANIGUCHI⁵, BERND BESCHOTEN¹, CHRISTOPH STAMPFER^{1,2}, and ANNIKA KURZMANN^{1,6} — ¹JARA-FIT and 2nd Institute of Physics A, RWTH Aachen University, Germany — ²Peter Grünberg Institute, FZ Jülich, Germany — ³AMO GmbH, Aachen, Germany — ⁴Research Center for Functional Materials, NIMS, Japan — ⁵International Center for Materials Nanoarchitectonics, NIMS, Japan — ⁶Physics Institute 2, University of Cologne, Germany

Two-dimensional hexagonal boron nitride is a host material for bright and stable single-photon emitters. By applying strain or electric fields, their emission properties can be tuned, rendering them promising candidates for quantum photonic applications [1,2]. Here, we present voltage-dependent photoluminescence measurements of a quantum emitter in dual-graphene-gated hBN, showing a gate-controllable, step-like, fivefold increase in emission intensity. Furthermore, we observe a correlation between the reported increase of emitter intensity and the direction of the leakage current through the hBN. This suggests photo-induced tunneling processes within the hBN as an explanation for the observed intensity switching. Thus, our results are a step towards understanding the charge dynamics between graphene gates and hBN quantum emitters.

- [1] Nano Lett. 18, 4710 (2018)
- [2] Light: Science & Applications 11, 186 (2022)

HL 26.5 Wed 10:30 EW 201

Excited state geometry relaxation of point defects in monolayer hexagonal boron nitride — ●ALEXANDER KIRCHHOFF, THORSTEN DEILMANN, and MICHAEL ROHLFING — University of Münster, Institute of Solid State Theory, Wilhelm-Klemm-Straße 10, 48149 Münster

Point defects in hexagonal boron nitride (hBN) are often discussed as single-photon emitters for quantum technologies. Understanding the dependence of electronic and optical properties on the geometry might help to identify the atomic structure of the defects and is also crucial in order to make these emitters applicable. Here, we study three defects in a monolayer of hBN, namely $C_B V_N$, $C_B C_N$ and $C_B O_N$, from an ab initio approach. We use (constrained) density functional theory to obtain optimal geometries of the electronic ground state and the first excited state, and then refine quasi-particle energies and optical excitation energies using a *GW* and BSE based approach. All three defect systems host transitions between deep lying defect states. We find the lowest defect exciton of $C_B C_N$ at ~ 4 eV and for the other two defects at ~ 2 eV with significant Stokes shifts of 0.2 eV and 0.7 eV, respectively.

HL 26.6 Wed 10:45 EW 201

Understanding the Role of Defects in WS₂ layer in contact with ZnO substrate — ●DEDI SUTARMA and PETER KRATZER — Department of Physics, University of Duisburg-Essen

The remarkable properties of two-dimensional (2D) materials have garnered significant attention in recent years, and understanding their fundamental behavior is critical for developing next-generation technologies. In this study, we investigate the microscopic behavior of a 2D material, WS₂, with ZnO (1 -1 0 0) taking the role as the substrate as well as charge injection layer in this van der Waals (vdW) heterostructures. Using density functional theory calculations, we examine the structural and optoelectronic properties of the WS₂/ZnO, including the impact of point defects. Herein, band alignment of the heterojunction is found to be type I, with the larger band gap in ZnO, which is desirable for using ZnO as an electron injector for radiative recombination in monolayer WS₂ forming the active layer in a light-emitting device. Our results demonstrate that defects can significantly modulate the electronic properties of the interface, including band alignment and charge transfer. Furthermore, absorption and Raman spectra are

calculated to understand the optical behavior of this system. This work is funded by DFG IRTG 2803 and NSERC CREATE.

15 min. break

HL 26.7 Wed 11:15 EW 201

Enhanced light-matter interaction in self-assembled photonic-defect nanocavities with a TMDC monolayer as active material — ●ARIS KOULAS-SIMOS¹, CHIRAG PALEKAR¹, KARTIK GAUR¹, IMAD LIMAME¹, CHING-WEN SHIH¹, BÁRBARA ROSA¹, CUN-ZHENG NING², and STEPHAN REITZENSTEIN¹ — ¹Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — ²Department of Electronic Engineering, Tsinghua University, Beijing 100084, China

Micro- and nanolasers utilizing TMDCs as active materials have been gaining significant research popularity for novel photonic applications. Here, we report on the fabrication of multiple self-assembled photonic-defect nanocavities in a single, fully encapsulated WSe₂ monolayer embedded in a dielectric distributed Bragg reflector (DBR) structure. The bubble-like Gaussian defect nanocavities provide tight optical lateral confinement and produce diameter-dependent optical signatures distinguishing them from the planar DBR-section, as validated in μ PL-measurements and numerical cavity simulations. Last but not least, optical power-dependent studies at cryogenic temperatures reveal an enhanced light-matter-interaction through a pronounced kink in the I/O-curve and a slight linewidth narrowing for two specific devices.

HL 26.8 Wed 11:30 EW 201

Optoelectronic energy conversion based on atom scale and sustainable device architectures — ●MAXIMILIAN A. GRUBER, ALEXANDER HÖTGER, and ALEXANDER W. HOLLEITNER — Walter-Schottky-Institute, TU Munich

Two-dimensional (2D) materials and heterostructures allow the exploration of fundamental quantum phenomena and advancing optoelectronics. Our work showcases a methodology for the integration of atomistic defects into 2D heterostructures, aiming to address the open-circuit voltage of single to few defects in a vertical tunneling device, revealing the potential of single-vacancy tunneling devices as atomic-scale photodiodes [1]. Moreover, we investigate the dynamics of hot charge carriers in atomically thin heterostructures via photocurrent and photovoltage experiments aiming to unravel the mechanisms of generation, transport and relaxation of hot carriers.

[1] A. Hötger *et al.* Photovoltage and photocurrent absorption spectra of sulfur vacancies locally patterned in monolayer MoS₂. Nano Letters accepted (2023)

HL 26.9 Wed 11:45 EW 201

Substrate-dependent quantum and magneto-optical properties of WSe₂ single-photon emitters — ●BÁRBARA ROSA¹,

CAIQUE SERATI DE BRITO², CESAR RICARDO RABAHI², INGRID D. BARCELOS³, YARA GALVÃO GOBATO², and STEPHAN REITZENSTEIN¹ — ¹Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — ²Department of Physics, Federal University of São Carlos, São Carlos, Brazil — ³Brazilian Synchrotron Light Laboratory, Brazilian Center for Research in Energy and Materials, Campinas, Brazil

Two-dimensional (2D) van der Waals materials have arisen as a novel platform to explore the characteristics of non-classical light throughout the fabrication of single-photon emitters (SPEs). Their large range of emission wavelengths, site-controllability, and the accessible properties tuning by engineered strain and defects, turning them into potential candidates for several applications. Here, we investigate the quantum-optical properties of WSe₂ SPEs generated on different substrates. Interestingly, by conducting off- and quasi-resonant optical excitation, we observe a substrate dependence on the number of quantum emitters and their extracted linewidths, in which the doped surfaces command the properties of defect-states created in WSe₂ SPEs. Similar effects are also observed in the multi-photon suppression determined through photon correlation measurements. In addition, we performed magneto-photoluminescence studies, where extracted g-factors for the systems above show a remarkably substrate-dependent response.

HL 26.10 Wed 12:00 EW 201

Monolayer-based single photon source in an open cavity featuring 65% brightness and quantum coherence — ●JENS-CHRISTIAN DRAWER¹, VICTOR NICOLAEVICH MITRYAKHIN¹, HANGYONG SHAN¹, SVEN STEPHAN^{1,2}, FALK EILENBERGER³, MARTIN SILIES², CARLOS ANTON-SOLANAS¹, MARTIN ESMANN¹, and CHRISTIAN SCHNEIDER¹ — ¹Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany — ²Hochschule Emden/Leer, Emden, Germany — ³Friedrich-Schiller-Universität Jena, Jena, Germany

In the fields of quantum communication and computation, non-classical light in the form of single photons is of critical importance. A promising candidate for single-photon sources are atomically thin crystals of layered van der Waals materials, although their performance has thus far been inferior to other state-of-the-art sources built from bulk crystals and semiconductors, such as InAs quantum dots. Here we present results from a single-photon source based on an atomically thin layer of WSe₂ coupled to an open-cavity optical resonator and operated at a temperature of 3.2K. A finely tuned cavity enables selective Purcell-enhanced emission with efficient quasi-resonant emitter excitation. We characterize its single-photon purity to be $g^{(2)}(0) = 0.047 \pm 0.007$, measured by the second-order coherence function $g^{(2)}$ in the Hanbury Brown and Twiss setup under pulsed operation, and observe a first-lens brightness of $65 \pm 4\%$ of linearly polarized photons. A first observation for this material, to our knowledge, was made in the form of quantum interference between successively emitted photons in a Hong-Ou-Mandel experiment.