CPP 32: 2D Materials IV (joint session HL/CPP)

Time: Wednesday 9:30–12:30 Location: POT 81

CPP 32.1 Wed 9:30 POT 81

Nonlinear optical characterization of atomically thin layers of the transition metal dichalcogenides WSe_2 and MoS_2 — •Henry Volker Hübschmann[1], Gerhard Berth[1], Ioannis Caltzidis[1], Katharina Burgholzer[2], Alberta Bonanni[2], and Klaus D. Jöns[1] — [1]Department of Physics, Paderborn University, 33098 Paderborn, Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, 4040 Linz, Austria

In the field of quantum technologies functional 2D-structures based on transition metal dichalcogenides like WSe_2 and MoS_2 represent a novel material platform due to their specific optical and electronic properties. In contrast to semimetallic graphene they feature an electronic band gap and a strong spinorbit coupling. Applications of such layered 2D-materials in functional structures are to be found within photonics, spinorbitronics or nanoelectronics. In this work we present our fundamental nonlinear study on mechanically exfoliated atomically thin layers of the semiconductors WSe_2 and MoS_2. In this context, the second harmonic generation was determined for both van der Waals layered material systems as a function of the layer number. The respective nonlinear behavior was proven by a power-dependent characterization and supplemented by polarimetric analysis. Nonlinear imaging of the flakes was successfully performed by confocal SH-microscopy. In a further step the oxidation of MoS_2 layered systems was analyzed, here it was shown that for an even number of layers the oxidation leads to a break of their centrosymmetric structure, which is manifested in the clear presence of a relatively strong second harmonic signal.

CPP 32.2 Wed 9:45 POT 81

Single Photon Emitters in hBN via ultra-low energy helium ion implantation — •Prokhor Tkhor[1,2], Minh Bui[1,2], Renu Rani[1], Thorsten Brazda[1], and Beata E. Kardynał[1,2] — [1]Peter Grünberg Institut-9, Forschungszentrum Jülich, Jülich — [2]Department of Physics, RWTH Aachen, Aachen

Properties of heterostructures of transition metal dichalcogenides depend strongly on the moire lattice configuration and on the strength of coupling between the constituent monolayers. The first one can be controlled by the lattice constant of the constituent monolayers and their relative orientation, while the latter can be tuned by changing the spacing between them. In this contribution, we study a heterostructure of monolayers of WSe2/ hBN/ WSe2 with a moire potential periodicity of around 5 nm. The insertion of a monolayer of hBN between the two WSe2 monolayers results in a weak coupling between them. We discuss the results of the measurements of the dependence of the photoluminescence on the doping and electric field in this system. In this system the lowest intralayer excitonic states are optically spin-forbidden and at low electron concentration the effect of the moire potential on scattering of electrons and excitons dominates the optical signal masking the effect of correlations. Further, we discuss the observed non-monotonic charge shifts between the monolayers as a function of applied electric field.

CPP 32.3 Wed 10:00 POT 81

Thin hexagonal boron nitride in the deep-UV: The pursuit of single photon emitters and their properties — •Nils Bernhardt[1], Luka Choi[1], Felix Nippert[1], Angus Gentle[2], Milos Toth[2], and Markus R. Wagner[1,3] — [1]Technische Universität Berlin, Berlin, Germany — [2]University of Technology Sydney, Sydney, Australia — [3]Paul-Drude-Institut, Berlin, Germany

Interest in hexagonal boron nitride (hBN) continues to grow in optoelectronics with the discovery of an increasing number of quantum emitters in all spectral ranges. The wide band gap and chemical stability inherent to this material encourage hBN as a semiconductor substrate, while the possibility of reliably fabricating thin films entails unusual and unique properties. Consequently, room-temperature defect quantum emitters with reproducible emission properties from the UV to the near-IR can be engineered for applications such as quantum communication.

In this work, we investigate the recently observed luminescence of hBN at 4.1eV with a pulsed, frequency-tripled titanium-sapphire laser at 240nm. Experimental methods such as photoluminescence spectroscopy and time-resolved fluorescence spectroscopy are utilized alongside a Hanbury Brown and Twiss interferometer for correlation measurements in the deep UV as a means to identify single-photon emitters. Through this approach, we are able to establish a scientific basis for further investigation into the UV emission of hBN.

CPP 32.4 Wed 10:15 POT 81

Electrical control of excitonic complexes in $MoSe_2$ homobilayers — •Bárbara Rosa[1], Chirag Palekar[1], Alisson Cadore[2], Yuhui Yang[1], Aris Koula-Simos[1], Sefaattin Tongay[3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Brazilian Nanotechnology National Laboratory, Campinas, Brazil — [3]School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, USA

Effects of periodic Moiré potential in transition metal dichalcogenides (TMDs) bilayers are directly controlled by the twist angle between the monolayers. Novel features arising from intra- and interlayer excitons, such as their ultrafast formation and charger transfer, long population recombination lifetimes, and binding energy of dozens of meVs, turn TMD heterostructures into an attractive device for the study and manipulation of optical and transport properties via electrical fields. Moreover, such effects may appear even more pronounced at twisted homobilayers, since the absence of lattice mismatch promotes the appearance of larger Moiré superlattices. In this work, we explore the ability to control excitonic complexes in $MoSe_2/MoSe_2$ twisted bilayers (t-BLs) by performing gate-dependent microphotoluminescence (μPL) spectroscopy at room temperature. We observe the energy tunability of several meVs occurring at the emission of excitonic complexes derived from the t-BL region. In addition, other effects, such as the emergence of new excitonic features, are observed through μPL spectroscopy at cryogenic temperatures.

15 min. break

CPP 32.5 Wed 10:45 POT 81

Tailoring Coulomb interactions in WS_2-graphene heterostructures — •David Tebbe[1], Marc Schütte[1], Kenji Watanabe[2], Takashi Taniguchi[3], Christoph Stampfer[1], Bernd Beschoten[1], and Lutz Waldecker[1] — [1]2nd Institute of Physics A, RWTH Aachen University — [2]Research Center for Functional Materials, Japan — [3]International Center for Materials Nanoarchitectonics, Japan

The exciton binding energy and the quasiparticle bandgap in two dimensional semiconductors depend on their dielectric environment.

We investigate the screening of Coulomb interactions in heterostructures of WS_2 and graphene, separated through thin spacer layers of hexagonal boron nitride (hBN). By using hBN spacers from one to 16 atomic layers, we experimentally determine the tuning of the exciton binding energy and the quasiparticle bandgap as a function of the WS_2-to-graphene interlayer spacing.

This change in both energies is well described by a one over distance dependence, which is consistent with a screening arising from an image charge induced by the graphene layer.

Additionally, by doping the graphene with a graphitic back gate, we show that the ability of the graphene to screen Coulomb interactions in neighbouring layers is strongly modified. We determine the change in screening strength to be approximately 20% at room temperature, demonstrating that Coulomb-interactions in WS_2 can be modified in-situ without changing the doping level of the material itself.

CPP 32.6 Wed 11:00 POT 81

Evidence for equilibrium exciton condensation in monolayer WTe2 — •Massimo Rontani — CNR-NANO, Modena, Italy

We present evidence [1] that the two-dimensional bulk of monolayer WTe2 contains electrons and holes bound by Coulomb attraction, excitons, that spontaneously form in thermal equilibrium. On cooling from room temperature to 100 K, the conductivity develops a V-shaped dependence on electrostatic doping, while the chemical potential develops a step at the neutral point. These features are much sharper than is possible in an independent-electron picture, but they can be accounted for if electrons and holes interact strongly and are paired in equilibrium. Our calculations from first principles show that the exciton binding energy is larger than 100 meV and the radius as small as 4 nm, explaining their formation at high temperature and doping levels.

Below 100 K, more strongly insulating behaviour is seen, suggesting that a charge-ordered state forms. The observed absence of charge density waves in this state is surprising within an excitonic insulator picture, but we show that it can be explained by the symmetries of the exciton wavefunction. Therefore, in addition to being a topological insulator, monolayer WTe2 exhibits strong correlations over a wide temperature range.

This work is done in collaboration with Elisa Molinari, Daniele Varsano, Samaneh Ataei, Maurizia Palummo, Bosong Sun, David Cobden. It is partially funded by MUR PRIN2017 No. 2017BZPKSZ EXC-INS and MaX EU Center of Excellence.

[1] B. Sun et al., Nature Physics 18, 94-99 (2022).

CPP 32.7 Wed 11:15 POT 81

Charge and exciton quenching at defect states in TMDC-graphene heterostructures — •Daniel Hernangómez-Pérez[1], Amir Kleiner[1], Andrea Donarini[2], and Sivan Refaely-Abramson[1] — [1]Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, 7610001 Rehovot, Israel — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

In recent years, studies of charge transfer and excitonic properties of van der Waals heterostructures have revealed a fertile research arena, spanning Coulomb blockade physics [1], ultrafast interlayer charge separation [2] or graphene-quenched photoluminescence [3]. We theoretically study charge transfer and excitonic properties in XS_2-graphene (X = W, Mo) heterobilayers with monoatomic chalcogen vacancies [4-5]. We discuss the impact of the subgap defect-based features in the microscopic dynamics, as well as the interplay between spatial symmetries and the spin degree of freedom through the spin-orbit interaction. Finally, we report the electronic and optical properties computed by many-body perturbation theory and show how defects and graphene alter the absorption properties of the TMDC due to a combination of folding, commensuration and impact of defect in-gap energy bands.

[1] N. Papadopoulos, *et al.* Phys. Rev. B 101, 165303 (2020). [2] S. Aeschlimann, *et al.* Science Advances 6 (20)(2020). [3] E. Lorchat, *et al.*, Nat. Nano. 15, 283 (2020). [4] D. Hernangómez-Pérez, A. Donarini, and S. Refaely-Abramson, arXiv:2209.14420. [5] D. Hernangómez-Pérez, A. Kleiner, and S. Refaely-Abramson (in preparation).

15 min. break

CPP 32.8 Wed 11:45 POT 81

The influence of anisotropy on excitons in magnetic semiconductors — •Marie-Christin Heissenbüttel, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Understanding the peculiar interrelation between crystal structure, magnetic properties and light-matter interaction in semiconducting two-dimensional-like magnets is of fundamental interest. From our ab-initio *GW*/Bethe-Salpeter equation calculations, we are able to examine electronic and excitonic properties on the same footing.

Because of its large crystal anisotropy combined with in-plane ferromagnetism, the van-der-Waals stacked CrSBr has recently come to the fore e.g. to study correlated phenomena. Due to the unique interplay of anisotropy, two-dimensional magnetism and optoelectronic properties resulting in a quantum confinement, we observe very flat dispersions, different effective masses and a quasi-1D behaviour of excitons within a monolayer of CrSBr [1]. Moreover, we find that the Rydberg series of two excitonic states is intricately modified by the different extension of the wavefunctions within momentum space.

[1] https://arxiv.org/abs/2205.13456

CPP 32.9 Wed 12:00 POT 81

From $MoSe_2$ to MoS_2 and everything in-between — •Jennifer Schmeink, Vladislav Musytschuk, Nicolas Hille, Erik Pollmann, Peter Kratzer, and Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik, Germany

Asymmetrical, or Janus transition metal dichalcogenide (TMDC) monolayers such as MoSSe are a current hot topic in the field of two-dimensional (2D) materials due to their unique properties. The most common approach of fabrication is to start off from one of the two base TMDCs' monolayer and selectively substitute the top-most layer of chalcogen atoms with another kind. However, if the substitution is partial, the resulting material resembles more an alloy than a Janus-type structure. These in-between materials show their own interesting features, as they allow for example a fluid optical bad-gap tuning from that of $MoSe_2$ at 1.54 eV over 1.70 eV for MoSSe up to 1.84 eV of MoS_2. In my talk I want to show off the varying optical and electronic properties of these $MoS_{2(1-x)}Se_{2x}$ ($0 \leq x \leq 1$) structures with a special focus on the Janus-type MoSSe monolayer. This talk will explore the fascinating question of what lies in between.

CPP 32.10 Wed 12:15 POT 81

Optimized Irradiation Protocol for Quantum Sensors in Hexagonal Boron Nitride — •Paul Konrad[1], Andreas Gottscholl[1], Andreas Sperlich[1], Igor Aharonovich[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, Julius-Maximilians-University of 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 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 an irradiation protocol for creation of V_B^- by nitrogen ions, leading to optimized spin relaxation parameters and therefore improving quantum metrology limits. We also present tremendous improvement of ODMR contrast showing hyperfine interaction on flakes of down to 80nm thickness.

[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).