CPP 5: 2D Materials I (joint session HL/CPP)

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

CPP 5.1 Mon 9:30 POT 81

Spin-valley physics in strained transition metal dichalcogenides monolayers — •Paulo E. Faria Junior[1], Klaus Zollner[1], Tomasz Woźniak[2], Marcin Kurpas[3], Martin Gmitra[4], and Jaroslav Fabian[1] — [1]University of Regensburg, Regensburg, Germany — [2]Wroclaw University of Science and Technology, Wroclaw, Poland — [3]University of Silesia, Chorzów, Poland — [4]Pavol Jozef Šafárik University in Košice, Košice, Slovakia

Transition metal dichalcogenides (TMDCs) are ideal candidates to explore the manifestation of spin-valley physics under external stimuli. Here, we investigate the influence of strain on the spin, orbital angular momenta and g-factors of monolayer TMDCs within first principles[1]. Our calculations reveal the behavior of direct exciton g-factors under the isolated impact of strain: tensile (compressive) strain increases (decreases) the absolute value of g-factors. Strain variations of 1% modify the bright (A and B) exciton g-factors by 0.3 (0.2) for W (Mo) based compounds and the dark exciton g-factors by 0.5 (0.3) for W (Mo) compounds, suggesting that strain can be responsible for g-factor fluctuations observed experimentally. We complete our analysis for the Gamma and Q valleys, revealing that the spin degree of freedom dominates. This fundamental microscopic insight into the role of strain in the spin-valley physics of TMDCs is crucial to understand recent experiments[2,3]. [1] Faria Junior et al., NJP 24, 083004 (2022). [2] Covre, Faria Junior et al., Nanoscale 14, 5758 (2022). [3] Blundo, Faria Junior et al., PRL 129, 067402 (2022). Funding: DFG SFB 1277, SPP 2244.

CPP 5.2 Mon 9:45 POT 81

A bright single-photon source based on a WSe_2 monolayer in an open cavity — •Victor Mitryakhin[1], Hangyong Shan[1], Jens-Christian Drawer[1], Sven Stephan[1], Martin Silies[2], Falk Eilenberger[3], Carlos Antón-Solanas[1], Martin Esmann[1], and Christian Schneider[1] — [1]Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany — [2]Hochschule Emden/Leer, 26723 Emden, Germany — [3]Friedrich-Schiller-Universität Jena, 07745 Jena, Germany

Single photon sources based on crystalline defects present in transition-metal dichalcogenide monolayers, 2D atomically thin direct-bandgap semiconductors, have recently emerged as a promising platform for realization of and use in quantum communication and information processing.

In this work, we investigate the properties of single photon emission from a single exciton in a WSe_2 monolayer weakly coupled to an asymmetric plano-concave microcavity consisting of freely movable mirrors in 3 directions. In this regard, it enables us for an in-situ control of the properties of the emission and the extraction efficiency of single photons in the device.

We report a highly bright and linearly polarized single photon source with source brightness exceeding 70 % under saturation conditions, polarization degree of 98.4±1.3 % and high photon purity noted by the second-order correlation $g^{(2)}(0)$ value of 0.047±0.007, measured in Hanbury-Brown-Twist type of a setup.

CPP 5.3 Mon 10:00 POT 81

Strong coupling of excitons in a WS2-monolayer coupled to a silver nanogroove array — •Yuhao Zhang[1], Hans-Joachim Schill[1,2], Stephan Irsen[2], and Stefan Linden[1] — [1]Physikalisches Institut, Universität Bonn — [2]Center of Advanced European Studies and Research (caesar)

In this work, we report on room-temperature interaction of a WS2 monolayer with a tapered nanogroove array milled into monocrystalline silver flake. The bare nanogroove array features three polariton branches resulting from the coupling of localized surface plasmon modes (LSPR) in the nanogrooves and propagation surface plasmon modes (SPP). The linewidth of the lower plasmon polariton branch critically depends on the geometry of the nanogrooves. When a WS2 monolayer is deposited on the nanogroove array with optimized damping, the reflection spectra show an avoided crossing of the exciton mode and the lower plasmon polariton branch with a Rabi splitting of 38.7 meV indicating strong exciton-plasmon polariton coupling.

CPP 5.4 Mon 10:15 POT 81

Theory of exciton localization in TMDCs using metal nanoparticles — •Robert Salzwedel[1], Lara Greten[1], Stefan Schmidt[1], Chelsea Carlson[2], Stephen Hughes[2], Malte Selig[1], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany — [2]Department of Physics, Queen's University, Kingston, Ontario, Canada

In recent years, monolayers of transition metal dichalcogenides (TMDCs) have attracted considerable attention due to their strong Coulomb and light-matter interactions, leading to tightly bound excitons with large optical oscillator strength. Due to the finite thickness of the monolayers, these excitons are very sensitive to the environment, which allows their properties to be tailored, e.g., by functionalization with molecules or metal nanoparticles (MNPs) [1,2].

We present a theory based on a self-consistent solution of Maxwell's and Bloch equations to analytically study a coupled system of MNP plasmons and TMDC excitons. For the combined system, we identify an effective eigenvalue equation that governs the center of mass motion of the dressed excitons in a plasmon-induced potential. Examination of the ensuing plexcitonic equation reveals the existence of bound states, which we interpret as excitons localized in the external potential. The appearance of these bound states in this potential is an indicator of strong coupling between excitons and plasmons.

[1] Carlson et al. (2021). PRB, 104(12), 125424.
[2] Denning et al. (2022). PRB, 105(8), 085306.

15 min. break

CPP 5.5 Mon 10:45 POT 81

Electronic effects of non-uniformly strained 2D TMDCs — •Mohammadreza Daqiqshirazi and Thomas Brumme — Chair of Theoretical Chemistry, Technische Universität Dresden, Bergstraße 66c, 01069 Dresden, Germany

Strain plays an important role in most 2D materials since there is a strong influence of the strain state on the relative band alignment of different valleys in the electronic band structure. The effects of non-uniform strain on the properties of 2D materials are scarcely studied theoretically, even if in experiments a lot of different structures can be found in which a spatial varying strain state is present such as wrinkles or folds. Here, we are investigating how such non-uniform strain influences the electronic properties of the prototypical 2D materials WSe2 and MoS2.We study nanoscale wrinkles and nanotubes in detail and discuss important differences in the strain distribution and magnitude, also to understand if nanotubes could be used as a model system for non-uniformly strained systems. Using Density Functional Theory we find that the inclusion of spin-orbit interaction is crucial to correctly predict the changes in the band structure of wrinkled 2D materials as the non-uniform strain changes the symmetry compared to a flat layer. This introduces a strong Rashba-like splitting of the valence-band maximum near the Γ point. The situation complicates even more with the addition of an extra layer forming a bilayer or a hetrobilayer. The spatial varying band alignments in wrinkled multilayers can lead to new interlayer excitons which are confined to certain regions of the system.

CPP 5.6 Mon 11:00 POT 81

Optical properties of monolayer $ReSe_2$ and ReS_2 — •Thorsten Deilmann — Institute of Solid State Theory, University of Münster, Germany

Rhenium-based transition metal dichalcogenides unite the fascinating characteristics of the confined in-plane physics with their reduced crystal symmetry. This paves the way for polarization-sensitive applications, such as optical logic circuits operating in the infrared spectral region.

Here, we investigate the doping-dependent optical properties of $ReSe_2$ and ReS_2 from first principles. Besides strong excitonic effects, recent experimental studies have reported three-particle states (i.e. trions) with trion binding energies of more than 100 meV [1,2]. Using our ab initio methods we are able to predict neutral and charged properties and find much smaller binding energies compared to experiment.

[1] Advanced Functional Materials, 10, 1905961 (2019)
[2] Applied Physics Letters 119, 113103 (2021)

CPP 5.7 Mon 11:15 POT 81

Evaluating Atomically Thin Single-Photon Sources for Quantum Key Distribution — •Timm Gao[1], Martin v. Helversen[1], Carlos Anton-Solanas[2], Christian Schneider[2], and Tobias Heindel[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

Quantum light sources are considered key building blocks for future quantum communication networks. In recent years, atomic monolayers of transition metal dichalcogenides (TMDCs) emerged as a promising material platform for the development of compact quantum light sources. In this work, we evaluate for the first time the performance of a single-photon source (SPS) based on a strain engineered WSe_2 monolayer [1] for applications in quantum key distribution (QKD) [2]. Employed in a QKD-testbed emulating the BB84 protocol, an antibunching of $g^{(2)}(0) = 0.127 \pm 0.001$ and a raw key rate of up to (66.95 ± 0.10)kHz make this source competitive with previous SPS based QKD experiments using quantum dot based SPSs. Furthermore, we exploit routines for the performance optimization previously applied to quantum dot based single-photon sources [2]. Our work represents an important step towards the application of TMDC-based devices in quantum technologies.

[1] L. Tripathi et al., ACS Photonics 5, 1919-1926 (2018)
[2] T. Gao et al., arXiv:2204.06427 (2022)
[3] T. Kupko et al., npj Quantum Information 6, 29 (2020)

CPP 5.8 Mon 11:30 POT 81

Theory of Thermalization of Excitons at Elevated Densities in Atomically Thin Semiconductors — •Manuel Katzer, Andreas Knorr, and Malte Selig — Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Atomically thin semiconductors exhibit tightly bound electron-hole pairs which stimulated exciton research in recent years [1]. So far, many studies focused on the understanding of exciton dynamics in the limit of very dilute systems. Recent experimental findings [2] raised the question of the excitonic thermalization behaviour for densities above this dilute, classical limit. Due to the co-bosonic nature of excitons [3], we find both bosonic but also fermionic contributions to the thermalization, with the fermionic Pauli blocking effects being dominant for a broad range of parameters. Based on a Heisenberg equation of motion ansatz [4], we discuss the first order of non-linear exciton-phonon interaction exceeding the classical Boltzmann scattering limit, in order to analyze the character of the exciton thermalization at elevated excitation densities.

[1] Wang et al. RMP 90, 021001 (2018). [2] Sigl et al. PRR 2 (4), 042044 (2020). [3] Katsch et al., PRL 124 25 257402 (2020). [4] Selig et al. PRR, 1, 022007 (2019).

15 min. break

CPP 5.9 Mon 12:00 POT 81

Strong exciton-plasmon coupling in hybrids of 2D semiconductors and plasmonic crystals — •Lara Greten[1], Robert Salzwedel[1], Stephen Hughes[2], Malte Selig[1], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany — [2]Department of Physics, Queen's University, Kingston, Canada

Monolayers of transition metal dichalcogenides (TMDCs) are direct-gap semiconductors that exhibit tightly bound excitons with pronounced optical amplitudes. Thus, they are promising for various optoelectronic applications and an excellent material to investigate excitons. Another material with a large optical amplitude is a plasmonic crystal - arrays of metal nanoparticles - which supports collective plasmon modes, and yields amplification of the electric fields on the nanoscale.

Here, we theoretically consider exciton-plasmon coupling in a hybrid structure of a TMDC layer interacting with a plasmonic crystal with a 2d lattice. Our study reveals a hybridization of plasmons and initially momentum dark excitons. In addition, we find an excitonic mode with negligible coupling to the plasmonic near field, emitting undisturbed radiation into the far field. To connect to related experiments, we compute the scattered light in the near- and far-field explicitly and identify signatures of strong exciton-plasmon coupling with a Rabi splitting of more than 100 meV. We also find that the uncoupled exciton mode results in a third peak at the undisturbed exciton energy.

CPP 5.10 Mon 12:15 POT 81

Enhancement of Light Emission in Hexagonal Boron Nitride Structures — •Felix Schaumburg, Marcel Zöllner, Vasilis Dergianlis, Stephan Sleziona, Marika Schleberger, Axel Lorke, Martin Geller, and Günther Prinz — Faculty of Physics and CENIDE, University Duisburg-Essen, Germany

Optical spectroscopy, especially Raman- and photoluminescence (PL)-spectroscopy, is commonly used to study the optical properties of 2D materials. In order to obtain the highest Raman/PL-signals, it is important to reduce the reflection of the excitation laser.

We studied a number of exfoliated hexagonal Boron Nitride (hBN) flakes with different thicknesses on a Si substrate with a 300 nm SiO_2 top layer. By changing the hBN layer thickness, we found a specific thickness, where all Raman signals (from Si, SiO_2 and hBN) showed maximum intensity, whereas the backscattered laser light was suppressed. To explain the increased intensities, we calculated the reflectivity and transmissivity of the full layer system (air, hBN, SiO_2, Si) for different hBN layer thicknesses and for different excitation wavelengths (457 nm, 532 nm, 633 nm), using the transfer-matrix-algorithm. To compare theory with experiment, we performed Raman measurements with the 3 different wavelengths on different flakes and determined their thicknesses with AFM-measurements.

Our results are in good agreement with theory and show that it is possible to choose the best flakes for spectroscopy, just by looking at their color in an optical microscope. This also allows us to easily find good flakes for observation of efficient single defect emission.