HL 20: 2D semiconductors and van der Waals heterostructures II (joint session HL/DS)

Time: Monday 15:00–18:30 Location: POT 81

Invited Talk HL 20.1 Mon 15:00 POT 81

Resonantly hybridized excitons in moiré superlattices in van der Waals heterostructures — •Alexander Tartakovskii — Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK

Recent years have seen significant effort in exploration of monolayer semiconductors such as transition metal dichalcogenides (TMDs) MoS_2, WS_2, $MoSe_2$, WSe_2 etc. Atomically-thin layers of two-dimensional materials can be assembled in vertical stacks held together by relatively weak van der Waals forces, allowing for coupling between monolayer crystals with incommensurate lattices and arbitrary mutual rotation. The lattice constant difference and the mutual rotation angle present new degrees of freedom for the design of novel meta-materials.

A profound consequence of using these new degrees of freedom is the emergence of an overarching periodicity in the local atomic registry of the constituent crystal structures, known as a moiré superlattice. Here, we show that in semiconducting heterostructures built of incommensurate $MoSe_2$ and WS_2 monolayers, excitonic bands can hybridize, which results in the resonant enhancement of the moiré superlattice effects. $MoSe_2$ and WS_2 are specifically chosen for the near degeneracy of their conduction band edges to promote the hybridization of intra- and interlayer excitons. For $MoSe_2/WS_2$ heterostructures with almost aligned pairs of monolayer crystals, the resonant mixing of the electron states leads to amplified effects of the heterostructure's geometrical moiré pattern on the dispersion of the hybridised excitons.

HL 20.2 Mon 15:30 POT 81

Intralayer and interlayer exciton dynamics in WSe_2/WS_2 van-der-Waals heterostructure — •Manan Shah, Lorenz Maximilian Schneider, and Arash Rahimi-Iman — Department of Physics and Materials Sciences Center, Philipps-Universität, Marburg, 35032 Germany

The van-der-Waals heterostructures (vdW-HS) comprising atomically thin transition-metal dichalcogenides (TMDCs) provide an unprecedented level of freedom for bandgap engineering. However, the HSs give rise to more complex behaviour due to the change in effective dielectric screening, interlayer coupling strength, and moiré potential. The effectiveness of these parameters primarily depends upon the spacing, lattice constant mismatch, and the twist angle between the layers. The hybrid band structure of the vdW-HS system arising from the magnitude of these phenomena is not yet completely understood.

Here, we report a type-II WSe_2/WS_2 HS where the electrons accumulate in the WS_2 monolayer (ML) and the holes accumulate in the WSe_2 ML owing to charge transfer, giving rise to interlayer excitons. This tungsten-based HS is of particular interest due to the presence of energetically favourable spin-forbidden dark A-excitonic states and a strong excitonic binding energy. Our optical-spectroscopy results exhibit the intralayer excitons, intralayer phonon-assisted dark excitons, and interlayer excitons along with the emergence of new excitonic states with a large oscillator strength between the optical bandgap of the constituting MLs [M. Shah et al., *Semiconductors* (in press)].

HL 20.3 Mon 15:45 POT 81

Enabling tailored 2D materials by introducing 1D organic-inorganic perovskites with supramolecular intra-layer interactions — •Philip Klement[1], Natalie Dehnhardt[2], Chuan-Ding Dong[3], Samuel Bayliff[4], Julius Winkler[2], Peter J. Klar[1], Stefan Schumacher[3,5], Sangam Chatterjee[1], and Johanna Heine[2] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Germany — [2]Department of Chemistry and Material Sciences Center, Philipps-Universität Marburg, Germany — [3]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Germany — [4]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, USA — [5]College of Optical Sciences, The University of Arizona, Tucson, USA

One of the major current challenges in 2D materials* synthesis is the intentional design of building blocks to introducing superior chemical and physical properties. The limiting factor in this approach is the commonly-believed paradigm that in-plane covalent interactions are strictly necessary to form 2D materials, limiting the number of candidates. Here we show that individual single layers of 2D organic-inorganic perovskites with only 1D covalent intralayer-interactions exist. [BzA]3[BiCl5]Cl (BzA = benzylammonium) is exfoliated down to single layers and reveals extremely strong dimensional effects evidenced by a 0.4 eV shift of the photoluminescence between bulk and single layers. We demonstrate that already 1D covalent interactions render 2D materials possible.

HL 20.4 Mon 16:00 POT 81

Layer-dependent and time-resolved photoluminescence in hBN-encapsulated InSe — •Tommaso Venanzi[1,2], Himani Arora[1,2], Stephan Winnerl[1], Alexej Pashkin[1], Phanish Chava[1,2], Zahkar Kudrynskyi[3], Takashi Taniguchi[4], Kenji Watanabe[4], Artur Erbe[1], Amalia Patane[3], Manfred Helm[1,2], and Harald Schneider[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, UK — [4]National Institute for Material Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

In the last years van der Waals semiconductors have become a subject of intense research. Within this class of materials, InSe shows promising optical and electronic properties. Here we present the optical properties of thin flakes of InSe encapsulated in hBN. The encapsulation in hBN protects the InSe flakes from external contamination assuring long-term stability and reducing the disorder potential in the flake. We have studied the photoluminescence (PL) for different temperatures and number of InSe atomic layers. The relative weights of the exciton and electron-hole contributions to the PL emission are discussed using a lineshape analysis. Our model introduces a PL temperature to include the effects of the disorder potential on the PL emission. Furthermore, we observe a sharp increase of the PL lifetime while decreasing the number of layers. This is due to direct-to-indirect bandgap transition driven by the thickness of the InSe flake.

HL 20.5 Mon 16:15 POT 81

Optical Initialisation and Readout of Spin Defects in hBN — •A. Gottscholl[1], M. Kianinia[2], V. Soltamov[1], C. Bradac[2], C. Kasper[1], K. Krambrock[3], A. Sperlich[1], M. Toth[2], M. Dietz[1], I. Aharonovich[2], and V. Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]School of Mathematics and Physical Sciences, Inivertiy of Technology Sydney, Ultimo, NSW 2007, Australia — [3]Departomento de Fisica, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brazil

The concept of optically addressable spin states in solids is considered as a major building block of upcoming quantum technologies. While several candidates in 3D crystals including diamond and silicon carbide have been extensively studied, the identification of spin-dependent processes in 2D materials has remained elusive. Optically accessible spin states in hBN are already theoretically predicted, however, they have not been observed experimentally yet. We investigated a bright 850nm defect-related fluorescence in hBN with magnetic resonance techniques and identified it as a negatively charged boron vacancy V_B^-, possessing a spin triplet ground state and a zero field splitting of 3.5 GHz [1]. The defect shows an optically detected magnetic resonance signature at room temperature and can be optically spin polarized at lower temperatures. Our results constitute a leap forward in establishing two-dimensional hBN as a prime platform for scalable quantum technologies.

[1] Gottscholl et al., arXiv:1906.03774

HL 20.6 Mon 16:30 POT 81

Theory of optical absorption in monolayers of transition metal dichalcogenides — •Frank Lengers, Doris E. Reiter, and Tilmann Kuhn — Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm Str. 10, 48149 Münster

Monolayers of transition metal dichalcogenides are attractive materials for optoelectronics due to their strong exciton-light interaction. At the same time the interaction of excitons and phonons plays a crucial role in these systems leading to strong phonon-assisted processes in optical experiments.

In this contribution different theoretical methods for the computation of linear absorption spectra in monolayers of transition metal

dichalcogenides are investigated. To be specific, we consider the spectra of $MoSe_2$ using either a correlation expansion in 2nd or 4th Born Approximation or an approximation closely related to the time convolution less master equation used in the theory of open quantum systems. We show that the 2nd Born Approximation gives poor results for elevated temperatures due to the exceptionally strong exciton-phonon interaction. On the other hand the time convolution less approach gives suprisingly good results despite its simplicity when compared to higher-order correlation expansion. This rather easy method can therefore be readily applied to the class of atomically thin solids where strong carrier-phonon interaction plays a vital role.

30 min. break.

HL 20.7 Mon 17:15 POT 81

Band filling and cross quantum capacitance in ion gated semiconducting transition metal dichalcogenide monolayers — •Haijing Zhang[1,2], Christophe Berthod[2], Helmuth Berger[3], Thierry Giamarchi[2], and Alberto Morpurgo[2] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [2]University of Geneva, Geneva, Switzerland — [3]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Ionic liquid gated field-effect transistors based on semiconducting transition metal dichalcogenides are used to study a rich variety of extremely interesting phenomena, while important aspects of how charge carriers are accumulated in these systems remain elusive. Here we present a thorough analysis of charge accumulation in MoSe_2 and WSe_2 monolayers. We identify the conditions when the chemical potential enters different valleys in the monolayer band structure and find that an independent electron picture describes the occupation of states well. Unexpectedly, however, the same analysis of the experiments shows that the total device capacitance cannot be simply described in terms of the series connection of a geometrical capacitance and of a quantum capacitance given by C_Q=eˆ2/(dμ/dn), as commonly assumed. This unexpected behavior occurs because a cross quantum capacitance contribution is present, which originates physically from mutual screening of the electric field generated by charges on one plate from charges sitting on the other plate. Our findings reveal an important contribution to the capacitance of physical systems that had been virtually neglected until now.

HL 20.8 Mon 17:30 POT 81

Theory of Exciton-Electron Coupling in Two-Dimensional Semiconductors — •Frederik Schirdewahn[1], Dominik Christiansen[1], Andreas Knorr[1], Tommaso Venanzi[2], Stephan Winnerl[2], and Malte Selig[1] — [1]Technische Universität Berlin, Germany — [2]Helmholtz Zentrum Dresden-Rossendorf, Germany

The strong Coulomb interaction in monolayers of doped transition metal dichalcogenides (TMDCs) leads to the formation of tightly bound excitons and electron gas assisted exciton transitions (trions)[1,2]. Here we present a microscopic approach within the Heisenberg equation of motion formalism for the excitonic absorption including trion signatures[3]. We discuss the impact of doping density and temperature on the absorption spectrum. Additionally we present a joint experiment theory study for THz pump VIS probe experiments of doped monolayer $MoSe_2$, where we find a red shift of exciton and trion lines which we trace back to a heating of the electrons due to the THz pulse finding a good comparison between theory and experiment.

[1] G. Plechinger et al., Nat. Commun. 7, 12715 (2016)
[2] T. C. Berkelbach et al., Phys. Rev. B 88, 045318 (2013)
[3] A. Esser et al., phys. stat. sol. (b) 2, 317 (2001)

HL 20.9 Mon 17:45 POT 81

Bosonic Condensation in a hybrid monolayer MoSe2-GaAs-microcavity — •Max Waldherr[1], Nils Lundt[1], Martin Klaas[1], Simon Betzold[1], Matthias Wurdack[2], Anton Nalitov[3], Sefaattin Tongay[4], Elena Ostrovskaya[2], Alexey Kavokin[3], Sven Höfling[1,5], and Christian Schneider[1] — [1]Technische Physik, Physikalisches Institut and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Germany — [2]Nonlinear Physics Centre, Research School of Physics and Engineering, Australian National University, Canberra, Australia — [3]Physics and Astronomy School, University of Southampton, Highfield, Southampton, UK — [4]School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, Arizona, USA — [5]SUPA, School of Physics and Astronomy, St. Andrews, UK

We observe bosonic condensation in a hybrid exciton-polariton system in the strong-coupling regime, with monolayer MoSe2 and GaAs quantum well excitons collectively coupling to a Tamm-plasmon mode. The onset of condensation in the hybrid polariton branch manifests in a superlinear increase of its emission intensity, accompanied by a distinct collapse of the linewidth, a core sign of temporal coherence. At further increasing pumping powers, we observe a continuing blueshift of the resonance originating from particle interactions with uncondensed excitons in the reservoir states. The spin-polarized emission is a clear sign of valley-selective condensation.

HL 20.10 Mon 18:00 POT 81

Micro-photoluminescence studies of defects hosting localized excitons in single-layer MoS_2 — •Oleg Gridenco, Kathrin Sebald, Christian Tessarek, Martin Eickhoff, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, D-28359 Bremen, Germany

Beside to free excitons, single-layer transition metal dichalcogenides (TMDs) can also host localized excitons that are bound to defect states and emit with energies smaller than the free-exciton energy. These localized emission centres often appear in as-prepared samples after exfoliation, but they can also be created or enhanced at specific positions by local engineering. In this talk, we will introduce our recent progress in the study of point defects in single-layer MoS_2. Defects were introduced by scanning a Ga^+ ion beam over a certain area of a single-layer using a focused ion beam (FIB) machine. The number of defects was controlled by varying the Ga^+ ion dose. By performing low-temperature micro-photoluminescence (μPL) spectroscopy we investigate the emission properties of localized excitons. Moreover, we found that the intentionally generated defect-related emission centres dominate the optical spectra of MoS_2 at low temperatures. Additionally, light emitted from free or localized excitons needs to be efficiently collected. Here we will discuss how plasmonic nanostructures on top of single-layers are particularly well suited for enhancing the quantum yield of single-layer TMDs.

HL 20.11 Mon 18:15 POT 81

On-demand exchange and spin-orbit in bilayer graphene sandwiched between TMDC and ferromagnet — •Klaus Zollner[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Physics, P. J. Šafárik University in Košice, 04001 Košice, Slovakia

Van der Waals heterostructures offer great potential for future device applications. Bilayer graphene on a transition-metal dichalcogenide (TMDC) experiences strong proximity spin-orbit coupling (SOC) [1], and record spin lifetime anisotropies are achievable [2]. Moreover, one can turn ON and OFF the SOC in bilayer graphene with a gate voltage [3], and realize a spin-orbit valve [1]. Similarly, one can have on-demand proximity exchange in a bilayer graphene/ferromagnetic-insulator heterostructure [4],realizing an exchange valve. The logical next step is to combine both proximity effects, exchange and SOC in bilayer graphene sandwiched between TMDC and ferromagnet-insulator. In this talk, we will present our results of a time-reversal field effect valve in doubly proximitized bilayer graphene.

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[1] Gmitra et al., Phys. Rev. Lett. 119, 146401 (2017). [2] Omar et al., Phys. Rev. B 100, 155415 (2019). [3] Island et al., Nature 571, 85 (2019). [4] Zollner et al., N. J. Phys. 20, 073007 (2018).