O 9: Transition-Metal Dichalcogenides and Boron Nitride (HL with O/TT)

Time: Monday 11:45–13:00 Location: ER 270

O 9.1 Mon 11:45 ER 270

$\mathbf{k}\cdot\mathbf{p}$ theory for two-dimensional transition metal dichalcogenide semiconductors — •Andor Kormanyos and Guido Burkard — University of Konstanz

We present $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians (for a review see [1]) parametrised by ab initio density functional theory calculations to describe the dispersion of the valence and conduction bands at their extrema (the K, Q, Γ, and M points of the hexagonal Brillouin zone) in atomic crystals of semiconducting monolayer transition metal dichalcogenides. We review the parametrisation of the essential parts of the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians for MoS_2, $MoSe_2$, WS_2, and WSe_2, including the spin-splitting and spin-polarisation of the bands We use $\mathbf{k}\cdot\mathbf{p}$ theory to analyse:

i) optical transitions in two-dimensional transition metal dichalcogenides over a broad spectral range;

ii) to discuss magnetotransport properties of the charge carriers in the K and $-K$ valleys.

[1] A. Kormányos, G. Burkard et al, arXiv:1410.6666

O 9.2 Mon 12:00 ER 270

Coulomb-Induced Valley Coupling in Transition Metal Dichalcogenides — •Gunnar Berghäuser, Andreas Knorr, and Ermin Malic — Institut für Theoretische Physik, Nichtlineare Optic und Quantenelektronik, Technische Universität Berlin, Germany

Within a microscopic model we investigate the impact of Coulomb-induced intervalley coupling on the optical properties of transition metal dichalcogenides (TMDs). Our approach is based on the density matrix formalism and allows an analytical treatment of the excitonic absorption under the influence of intervalley coupling. We find that the strong Coulomb interaction in these atomically thin 2-dimensional materials couples resonant excitonic states in K and K' valleys [1]. This coupling leads to a splitting of excitonic absorption peaks in the range of the trion binding energy. We further investigate the impact of experimentally accessible parameters, such as doping, dielectric environment, and the detuning of resonant states in the K and K' valley, on the intervalley coupling. The gained insights are of crucial importance for the application of TMDs in valleytronics.

[1] Gunnar Berghäuser and Ermin Malic, "Analytical approach to excitonic properties of MoS_2", Phys. Rev. B 89, 125309 (2014)

O 9.3 Mon 12:15 ER 270

Coupled spin-valley-dynamics in singlelayer transition metal dichalcogenides — •Gerd Plechinger, Nicola Paradiso, Philipp Nagler, Sven Gelfert, Christoph Strunk, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

Single layers of transition metal dichalcogenides (TMDCs) like MoS_2 and WS_2 can be produced by simple mechanical exfoliation. Offering a direct bandgap at the K-points in the Brillouin zone, they represent a promising semiconductor material for flexible and transparent optoelectronic applications. Due to inversion symmetry breaking together with strong spin-orbit-interaction, the valley and spin degrees of freedom are coupled in singlelayer TMDCs. Via circularly polarized optical excitation, an efficient polarization of the K^+ or the K^- valley can be generated. Here, we optically investigate the dynamics of these coupled spin-valley polarizations in singlelayer MoS_2 and singlelayer WS_2 by means of time-resolved Kerr rotation (TRKR) and display the dependence of the spin lifetime on the temperature and the excitation energy. Moreover, we probe the influence of mild annealing on the lifetimes.

O 9.4 Mon 12:30 ER 270

Low-temperature photoluminescence of 2D Dichalcogenides and indirect excitons in their heterostructures — •Philipp Nagler[1], Gerd Plechinger[1], Philipp Tonndorf[2], Steffen Michaelis de Vasconcellos[2], Rudolf Bratschitsch[2], Christian Schüller[1], and Tobias Korn[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040, Regensburg, Germany — [2]Physikalisches Institut, Westphälische Wilhelms-Universität Münster, 48149, Münster, Germany

Two-dimensional transition-metal dichalcogenides (TMD) have recently emerged as a promising class of direct-gap semiconductors. Here, we present low-temperature photoluminescence (PL) measurements of four different monolayer TMDs, namely MoS_2, $MoSe_2$, WS_2 and WSe_2. The diselenides show a clear splitting of neutral exciton and trion which enables us to deduce the binding energy of the trion. Furthermore, by using a deterministic transfer technique we are able to fabricate van-der-Waals heterostructures consisting of different 2D TMDs. At room temperature, we observe indirect excitons at the interface which probably stem from a spatial separation of electrons and holes. Power-dependent PL measurements on the heterostructures allow us to alter the excitonic regime and to probe saturation effects of the system.

O 9.5 Mon 12:45 ER 270

Synthesis of atomically thin hexagonal boron nitride films on polycrystalline nickel substrates using MBE — •Siamak Nakhaie, Joseph M. Wofford, Timo Schumann, Uwe Jahn, João Marcelo Lopes, and Henning Riechert — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Hexagonal boron nitride (h-BN) has recently been the subject of an intense research effort. This has in large part been driven by the suitability of h-BN for integration into heterostructures with other 2-dimensional materials, such as graphene [1]. We report the synthesis of h-BN on polycrystalline Ni foils by molecular beam epitaxy (MBE) from elemental B and N. The presence of a well-ordered, crystalline h-BN film on the Ni foil substrate was confirmed using Raman spectroscopy, which revealed a sharp peak at 1365 cm^{-1}. The ubiquity of wrinkle structures in numerous atomic force microscopy scans, together with the uninterrupted observation of the h-BN Raman signal, offer strong evidence of a continuous h-BN film. Using shorter duration depositions we were able to gain insight into the nucleation and growth behavior of h-BN before forming a closed film. According to scanning electron microscopy (SEM) images, we observed the morphology of sub-monolayer h-BN islands to evolve from star-shaped to much larger compact triangles with increasing growth temperature. SEM micrographs also clearly showed points of increased contrast at the approximate geometric centers of the islands, suggesting that the h-BN nucleated heterogeneously. [1] C.R. Dean et al., Nat. Nanotechnol. 5 (2010) 722