O 57: Focus Session: Many-body effects in two-dimensional materials

Organizers: Christopher Gies and Tim Wehling (Universität Bremen)

Time: Wednesday 9:30–13:00 Location: H16

Invited Talk O 57.1 Wed 9:30 H16

Probing bandgap renormalization, excitonic effects, and interlayer coupling in 2D transition metal dichalcogenide semiconductors — •Miguel M. Ugeda[1], Aaron Bradley[1], Sufei Shi[1], Felipe H. Jornada[1], Yi Zhang[2,3], Diana Qiu[1], Wei Ruan[1], Sebastian Wickenburg[1], Alexander Riss[1], Jiong Lu[1], Sung-Kwan Mo[2], Zahid Hussain[2], Zhi-Xun Shen[3], Feng Wang[1], Steven G. Louie[1], and Michael F. Crommie[1] — [1]Department of Physics, University of California, Berkeley, CA 94720, USA. — [2]Advanced Light Source, Lawrence Berkeley National Lab., Berkeley, CA 94720, USA. — [3]Stanford Institute for Materials and Energy Sciences, Menlo Park, CA 94025, USA.

Reduced screening in 2D metal dichalcogenides (TMDs) has been predicted to result in dramatically enhanced Coulomb interactions that should cause giant bandgap renormalization and excitonic effects. Here we present direct experimental observation of extraordinarily high exciton binding energy and band structure renormalization in a single-layer of semiconducting TMD[1]. We have determined the binding energy of correlated electron-hole excitations in monolayer MoSe2 grown via molecular beam epitaxy on bilayer graphene by using a combination of scanning tunneling spectroscopy and photoluminescence spectroscopy. We have also studied the role of interlayer coupling and layer-dependent carrier screening on the electronic structure[2] of few layer MoSe2. We find that the electronic quasiparticle bandgap decreases by nearly 1 eV when going from one layer to three. [1]Nature Materials 13, 1091 (2014). [2]Nano Letters 15, 2594 (2015).

O 57.2 Wed 10:00 H16

A Tight Binding Approach to Strain and Curvature in Monolayer Transition-Metal Dichalcogenides — •Alexander Pearce and Guido Burkard — Department of Physics, University of Konstanz, D-78464 Konstanz, Germany

We present a model of the electronic properties of the monolayer transition-metal dichalcogenides based on a tight binding approach which includes the effects of strain and curvature of the crystal lattice. Mechanical deformations of the lattice offer a powerful route for tuning the electronic structure of the transition-metal dichalcogenides, as changes to bond lengths lead directly to corrections in the electronic Hamiltonian while curvature of the crystal lattice mixes the orbital structure of the electronic Bloch bands. We first present an effective low energy Hamiltonian describing the electronic properties near the K point in the Brillouin zone, then present the corrections to this Hamiltonian due to arbitrary mechanical deformations and curvature in a way which treats both effects on an equal footing. This analysis finds that local area variations of the lattice allow for tuning of the band gap and effective masses, where the application of uniaxial strain decreases the magnitude of the direct band gap at the K point. Additionally, strain induced bond length modifications create a fictitious gauge field but with a coupling that is smaller than seen in related materials like graphene. We also find curvature of the lattice leads to the appearance of both an effective in-plane magnetic field which couples to spin degrees of freedom and a Rashba-like spin-orbit coupling due to broken mirror inversion symmetry. (arXiv:1511.06254).

O 57.3 Wed 10:15 H16

Observation of charge density wave order in 1D mirror twin boundaries of single-layer MoSe2 — •Sara Barja[1], Sebastian Wickenburg[1], Zhen-Fei Liu[1], Yi Zhang[1], Hyejin Ryu[1], Miguel M. Ugeda[2], Zahid Hussain[1], Zhi-Xun Shen[3], Sung-Kwan Mo[1], Miquel B. Salmeron[1,2], Feng Wang[1,2], Michael F. Crommie[1,2], D. Frank Ogletree[1], Jeffrey B. Neaton[1,2], and Alexander Weber-Bargioni[1] — [1]Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [2]University of California at Berkeley, Berkeley, CA, USA — [3]Stanford Institute of Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA, USA

Detailed understanding of defect structure in 2D transition metal dichalcogenides may lead to control of the material properties. Here we provide direct evidence for the existence of isolated, 1D charge density waves (CDWs) at mirror twin boundaries (MTBs) in single-layer MoSe2. 4K-STM/STS measurements reveal a substantial bandgap of 60-140 meV opening at the Fermi level in the otherwise one dimensional metallic structure. We find an energy-dependent periodic modulation in the density of states along the MTB, with a wavelength of approximately three lattice constants. The modulations in the density of states above and below the Fermi level are spatially out of phase, consistent with CDW order. In addition to the electronic characterization, we determine the atomic structure and bonding configuration of the 1D MTB by means of high-resolution nc-AFM. DFT calculations reproduce both the gap opening and the modulations of the density of states.

O 57.4 Wed 10:30 H16

Probing the anisotropic interlayer Raman modes of few-layer ReS_2 — •Philipp Nagler, Gerd Plechinger, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040, Regensburg, Germany

ReS_2 has recently emerged as a new member in the rapidly expanding family of two-dimensional materials. Unlike MoS_2 or WSe_2, the optical and electrical properties of ReS_2 are not isotropic due to the reduced symmetry of the crystal. Here, we probe the anisotropic behavior of ReS_2 by Raman spectroscopy in the ultralow frequency regime. Thereby, we are able to access the layer breathing modes (LBM) and shear modes (LSM) of the material which stem from rigid-layer oscillations. The layer dependence of their peak positions enables an easy determination of the layer number of the crystal and can be readily reproduced by means of a monoatomic chain model. By varying the angle between the linearly polarized laser and the in-plane crystal axis, we are able to reveal an energetic shift of the LSM which is directly linked to the in-plane anisotropy of the shear modulus in this material.

30 min. Coffee Break

Invited Talk O 57.5 Wed 11:15 H16

Enhanced light-matter coupling and single-photon emission of atomically thin semiconductors — •Rudolf Bratschitsch — Westfälische Wilhelms-Universität Münster, Münster, Deutschland

Graphene is known as a prototypical two-dimensional material with unique physical properties. However, the difficulty of creating an optical band gap stimulated the search for other monolayer materials. In my talk I will show that atomically thin transition metal dichalcogenides serve as a promising new material class for opto-electronics and quantum optics [1-3]. In particular, I will explain, how gold nanoantennas may be used to increase the light-monolayer coupling and present single-photon emission from localized excitons in monolayer WSe2.

[1] P. Tonndorf et al., Optics Express 21, 4908 (2013)
[2] J. Kern et al., ACS Photonics 2, 1260 (2015)
[3] P. Tonndorf et al., Optica 2, 347 (2015)

Invited Talk O 57.6 Wed 11:45 H16

Optical Properties and Carrier Dynamics in Transition Metal Dichalcogenides — •Alexander Steinhoff-List[1], Malte Rösner[1,2], Matthias Florian[1], Michael Lorke[1], Christopher Gies[1], Ji-Hee Kim[3], Deok-Soo Kim[4], Chanwoo Lee[4], Gang Hee Han[3], Mun Seok Jeong[3,4], Tim Wehling[1,2], and Frank Jahnke[1] — [1]Institut für Theoretische Physik, Universität Bremen, P.O. Box 330 440, 28334 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, 28334 Bremen, Germany — [3]Center for Integrated Nanostructure Physics, Institute for Basic Science, Suwon 440-746, Republic of Korea — [4]Department of Energy Science, Sungkyunkwan University, Suwon 440-746, Republic of Korea

As two-dimensional transition metal dichalcogenides are promising candidates for optoelectronic applications, there is a strong interest in understanding the influence of excited carriers in these materials on optical properties. We present studies of absorption and photoluminescence spectra of monolayer MoS_2 in the presence of excited carriers as well as carrier kinetics, based on material-realistic ab-initio band structures and interaction matrix elements. It is shown that absorption spectra are strongly modified due to band-gap renormalization and

screening effects, while the photoluminescence signal can be distinctly influenced by optical excitation above or below the electronic band gap. Moreover, we present results for carrier-carrier Coulomb and carrier-phonon scattering after optical excitation of the monolayer, exhibiting ultra-fast carrier relaxation on the sub-100 fs time scale.

O 57.7 Wed 12:15 H16

Microscopic modeling of the homogeneous linewidth in absorption spectra of TMDs — •Malte Selig[1], Gunnar Berghäuser[2], Ermin Malic[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

Monolayer transition metal dichalcogenides (TMDs) are direct-gap semiconductors with strong light-matter and Coulomb interaction. The latter accounts for strongly bound excitons, which dominate the optical spectrum. Here, we investigate the homogeneous linewidth in excitonic spectra induced by radiative coupling and exciton-phonon scattering. In conventional semiconductors, the radiative dephasing / recombination is typically weak in comparison to the electron-phonon scattering which mainly determines the homogeneous linewidth. The situation turns out to be different in atomically thin TMDs. Based on the density matrix formalism combined with the tight-binding approximation, we explicitly calculate the dephasing rates stemming from exciton-radiation interaction and exciton-phonon scattering. We find that in TMDs the radiative coupling is in the range of 1 meV clearly exceeding the exciton-phonon rate. We systematically investigate the resulting homogenous linewidth in absorption spectra of the most prominent TMDs for different temperatures, dopings, and substrates. [1]

[1] Galan Moody et al. Nat Commun 6, 8315 (2015)

O 57.8 Wed 12:30 H16

Influence of the spin-orbit splitting on the coupled spin-valley-dynamics in monolayer transition metal dichalcogenides — •Gerd Plechinger, Philipp Nagler, Sven Gelfert, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

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 promising semiconductor materials 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 monolayer TMDCs. Via circularly polarized optical excitation, an efficient polarization of the K^+ or the K^- valley can be generated. Here, we investigate the dynamics of these coupled spin-valley polarizations in monolayer MoS_2 and WS_2 by means of photoluminescence spectroscopy and time-resolved Kerr rotation (TRKR). The results indicate a maximum achievable spin-valley-lifetime in these materials exceeding one nanosecond at low temperatures. Furthermore, we extract the dependence of the spin-valley lifetime on temperature. By varying the excitation energy, we reveal the excitonic resonances as well as the spin-polarized bandstructure around the K valleys common to monolayer TMDCs.

O 57.9 Wed 12:45 H16

Ultrafast Coulomb-induced intervalley coupling in atomically thin WS_2 — Robert Schmidt[1], •Gunnar Berghäuser[2], Malte Selig[3], Philipp Tonndorf[1], Ermin Malic[2], Andreas Knorr[3], Steffen Michaelis de Vasconcellos[1], and Rudolf Bratschitsch[1] — [1]Institute of Physics and Center for Nanotechnology, University of Münser, Münster Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden — [3]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Monolayers of semiconducting transition metal dichalcogenides hold the promise for a new paradigm in electronics by exploiting the valley degree of freedom in addition to charge and spin. For these materials valley polarization can be conveniently initialized and read out by circularly polarized light. However, the underlying microscopic processes governing the valley polarization in these atomically thin equivalents of graphene are still not fully understood. Here, we present a theoretical study on the ultrafast time-resolved intervalley dynamics in monolayer WS_2 [1]. Based on a microscopic theory, we reveal the many-particle mechanisms behind the observed spectral features. We show that Coulomb-induced intervalley coupling explains the immediate and prominent pump-probe signal in the unpumped valley as well as the seemingly low valley polarization degrees typically observed in pump-probe measurements if compared to photoluminescence studies.

[1] R. Schmidt et al, submitted (2015)