O 46: 2D semiconductors and van der Waals heterostructures IV (joint session HL/DS/O)

Time: Tuesday 14:00–16:00 Location: POT 81

O 46.1 Tue 14:00 POT 81

Resolving the interlayer charge transfer in van der Waals heterostructures by ultrafast THz emission nanoscopy — •Markus Plankl[1], Martin Zizlsperger[1], Fabian Mooshammer[1], Felix Schiegl[1], Fabian Sandner[1], Markus A. Huber[1], Tom Siday[1], Jessica L. Boland[2], Tyler L. Cocker[3], and Rupert Huber[1] — [1]Department of Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Photon Science Institute, University of Manchester, Manchester M13 9PL, UK — [3]Department of Physics and Astronomy, Michigan State University, 48824 Michigan, USA

In van der Waals heterostructures composed of two transition metal dichalcogenide monolayers, photogenerated electron-hole pairs are spatially separated on ultrafast timescales, giving rise to the formation of interlayer excitons. Yet, the underlying interlayer charge transfer has only been investigated in a spatially averaged manner. Consequently, probing nanoscale transfer efficiencies and tunneling rates has so far remained elusive. Since the tunneling of photoexcited charge carriers between adjacent layers represents an ultrafast current along the out-of-plane direction, a concomitant electromagnetic pulse in the terahertz spectral range is emitted. By combining electro-optic time-domain spectroscopy with near-field microscopy, we resolve this characteristic fingerprint of the interlayer carrier dynamics on the nanoscale with sub-cycle temporal resolution. Thereby, we infer tunneling characteristics, which we relate with the nanoscale conductivity of the heterostructure.

O 46.2 Tue 14:15 POT 81

Influence of dark states on excitonic spin relaxation in transition metal dichalcogenides — •Malte Selig, Dominik Christiansen, and Florian Katsch — Technische Universität Berlin, Berlin, Germany

Energetically low lying dark exciton states with momenta well above the radiative cone manifest a significant relaxation channel for optically pumped excitons in transition metal dichalcogenides (TMDCs). While they have been demonstrated to influence the optical linewidth [1], lineshape [2], relaxation and luminescence properties [3], they can also be expected to play a crucial role for the spin relaxation of excitons.

Here we present a Heisenberg equation of motion theory for the intervalley exchange coupling, mediating the spin relaxation, and exciton phonon coupling. We demonstrate that the interplay of both mechanisms leads to unintuitive signatures in pump probe experiments where the A transition is pumped and either A or B transition are probed [4]. Additionally we reveal that the presence of energetically low lying dark excitons significantly quenches the efficiency of intervalley exchange coupling [5]. Our theoretical results shine new light on existing experimental data.

[1] M. Selig et al.,Nature Commun. 7,13279 (2016)
[2] D. Christiansen et al., Phys. Rev. Lett. 119, 187402 (2017)
[3] M. Selig et al., 2D Mat. 5, 035017 (2018)
[4] M. Selig et al., Phys. Rev. Research 1, 022007(R) (2019)
[5] M. Selig et al., arXiv:1908.11178 (2019)

O 46.3 Tue 14:30 POT 81

Kelvin probe force microscopy-based direct measurements of contact resistance in 2D semiconductor thin film transistors — •Aleksandar Matkovic[1], Andreas Petritz[2], Gerburg Schider[2], Markus Krammer[4], Markus Kratzer[1], Michael Gärtner[3], Andreas Terfort[3], Christian Teichert[1], Egbert Zojer[4], Karin Zojer[4], and Barbara Stadlober[2] — [1]Institute of Physics, Montanuniversität Leoben, Leoben, Austria. — [2]Joanneum Research MATERIALS, Institute for Surface Technologies and Photonics, Weiz, Austria. — [3]Institute of Solid State Physics, Graz University of Technology, Graz, Austria. — [4]Institut für Anorganische und Analytische Chemie, Goethe-University Frankfurt, Frankfurt am Main, Germany.

This study aims at direct determination of the contact resistance in MoS_2-based thin film transistors (TFTs). Exfoliated single-crystal flakes of MoS_2 have been used in a bottom-contact TFT configuration. Pyrimidine-containing self-assembled monolayers (SAMs) were employed to tune the work function of gold electrodes. Kelvin probe force microscopy measurements were carried out during operation of the devices in order to directly image potential drops across the channel and to study the influence of different SAM treatments on the contact resistance. By independently imaging potential drops at both, carrier injection and extraction points, we demonstrate the asymmetry of contact resistances in MoS_2-based TFTs, as well as their non-linear and bias-dependent behavior.

O 46.4 Tue 14:45 POT 81

MOVPE of large-scale 2D-2D heterostructures for optoelectronic applications — Annika Grundmann[1], Clifford McAleese[2], Ben Richard Conran[2], Andrew Pakes[2], Dominik Andrzejewski[3], Tilmar Kümmel[3], Gerd Bacher[3], Kenneth Bo Khin Teo[2], •Michael Heuken[1,4], Holger Kalisch[1], and Andrei Vescan[1] — [1]Compound Semiconductor Technology, RWTH Aachen University, Aachen, Germany — [2]AIXTRON Ltd., Cambridge, United Kingdom — [3]Werkstoffe der Elektrotechnik and CENIDE, University Duisburg-Essen, Duisburg, Germany — [4]AIXTRON SE, Herzogenrath, Germany

Vertical heterostructures of two (or more) different 2D layer provide many fascinating opportunities by combining the unique intrinsic chemical, physical and (opto)electronic properties of 2D materials. Without the need of consideration of lattice matching, a nearly infinite number of potential combinations of 2D layers are possible. Transition metal dichalcogenide (TMDC) monolayers are the most widely studied 2D semiconductors beyond graphene and thus provide a strong basis for understanding the properties of 2D heterostructures. Unlike mechanical exfoliation, direct successive growth of 2D-2D heterostructures requires a controlled synthesis of the respective monolayers with pristine interlayer interfaces and no intermixing of disparate layers. Here, we report on direct successive MOCVD of vertical MoS_2-WS_2 and WS_2-MoS_2 heterostructures as well as MOCVD of WS_2 and MoS_2 onto graphene previously deposited in another MOCVD reactor.

O 46.5 Tue 15:00 POT 81

Efficient Hot Electron Transfer at Graphene-WS2 van der Waals Bilayers — SHuai Fu and •Hai Wang — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Hybridization of (semi-)metallic and semiconducting monolayers, such as graphene and layered transition metal dichalcogenides (TMDs), enables efficient and sensitive photodetectors, by combing the synergetic properties of strong absorption at exciton resonances in TMDs, efficient charge transfer cross the interfaces and ultrahigh charge mobility in graphene. In spite of the great advance in devices, the fundamental understanding of the mechanism underlying the ultrafast charge flow across the heterostructures lags far behind, and effective means of controlling its efficiency have not been established.

Employing Terahertz spectroscopy, we shed light on the fundamentals of ultrafast interfacial nonequilibrium dynamics in graphene-WS2 van der Waals bilayers. We report an efficient and ultrafast hot electron injection from graphene to WS2, which competes with hot carrier heating process in graphene. We will discuss the mechanism underlying the hot electron charge transfer process, and factors governing its efficiency and lifetime of interfacial charge states, which are critical for efficient optoelectronics (i.e. photodetectors) based on van der Waals heterostructures.

O 46.6 Tue 15:15 POT 81

Excitation Induced Dephasing in Monolayer Transition Metal Dichalcogenides — •Florian Katsch, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, 10623 Berlin, Germany

Exceptionally strong Coulomb interactions in atomically thin transition metal dichalcogenides lead to tightly bound electron-hole pairs (excitons) dominating their linear and nonlinear optical response. The latter involves bleaching [1], energy renormalizations [2], and higher-order Coulomb correlation effects like biexcitons [3] and excitation induced dephasing (EID) [4]. Whereas bleaching, energy renormalizations, and biexcitons are widely investigated, EID in exciton dominated semiconductors so far lacks microscopic calculations. Within a Heisenberg equations of motion formalism we identify the coupling between excitons and exciton-exciton scattering continua as the most prominent process causing EID and sideband formation. Evaluating

the EID for single-layers of transition metal dichalcogenides, we find a good agreement with recent experiments [5,6].

[1] M. Selig *et al.*, Physical Review Research **1**, 022007 (2019).
[2] J. Shacklette and S. Cundiff, Physical Review B **66**, 045309 (2002).
[3] E. Sie *et al.*, Physical Review B **92**, 125417 (2015).
[4] H. Wang *et al.*, Physical Review Letters **71**, 1261 (1993).
[5] G. Moody *et al.*, Nature Communications **6**, 8315 (2015).
[6] E. Martin *et al.*, arXiv preprint arXiv:1810.09834 (2018).

O 46.7 Tue 15:30 POT 81

Dirac physics in honeycomb semiconductors — •Christiaan Post[1], Nathali Franchina Vergel[2], Tomas Meerwijk[1], Jesper Moes[1], Xavier Wallart[2], Guillaume Fleury[3], Ludovic Desplanque[2], Ingmar Swart[1], Christophe Delerue[2], Bruno Grandidier[2], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht, The Netherlands — [2]Institute of Electronics, Microelectronics and Nanotechnology (IEMN), Lille, France — [3]Laboratory for Chemistry of Organic Polymers (LCPO), Bordeaux, France

III-V semiconductor quantum wells have obtained a central place in advanced logics and opto-electronics. In more recent research, the effects of a nano scale geometry forming a periodic scattering potential in the lateral directions of the quantum well have been discussed and calculated. In case of a nano-scale honeycomb geometry, Dirac cones are formed similar as for graphene, creating massless fermions while the semiconductor quantum well band gap remains nearly unaltered.

In this research, we report on the electronic characterization of a modulated InGaAs quantum well with a honeycomb symmetry. The honeycomb symmetry is fabricated by perforating the quantum well with a triangular symmetry using nano-scale lithography. By performing scanning tunneling microscopy experiments, the electronic properties of the sample are intensively investigated, showing the combined electronic properties of a two-dimensional material and Dirac-like features. Muffin-tin calculations support the obtained experimental results, revealing the exciting properties of these novel materials.

O 46.8 Tue 15:45 POT 81

Structural and electronic properties of twisted MoS_2 bilayers — •Somepalli Venkateswarlu, Andreas Honecker, and Guy Trambly de Laissardière — Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France

Vertically stacked transition metal dichalcogenides of multilayer structures have gained increasing attention because of their fascinating features in electronics and optical properties [1]. We performed calculations of structural and electronic properties of nontwisted and twisted MoS_2 bilayers using first-principle calculations [ABINIT][2] and the tight-binding (TB) method. Our results reveal significant differences in the band structures of twisted and nontwisted ones: the appearance of a crossover between direct and indirect band gap, gap variation, and atomic relaxations. For rather large angles, the band structures are very similar for different rotation angles [3]. For the smallest angles, TB calculations predict some flat bands in the valence band and conduction band. As in twisted bilayer graphene, the corresponding states are localized in the AA stacking region of the Moiré pattern.

[1] E. S. Kadantsev, P. Hawrylak, Solid State Comm. **152**, 909 (2012).

[2] X. Gonze *et al.*, Comp. Mat. Sci. **25**, 478 (2002). https://www.abinit.org.

[3] Z. Wang *et al.*, J. Phys. Chem. C **119**, 4752 (2015).