CPP 65: Two-dimensional Materials IV (joint session HL/CPP)

Time: Friday 9:30–13:00 Location: H36

CPP 65.1 Fri 9:30 H36

Optical Valleytronic Properties of CVD-grown Tungsten Disulfide AA' and AB Bilayers — •Lorenz Maximilian Schneider[1], Jan Kuhnert[1], Simon Schmitt[1], Ulrich Huttner[1], Lars Meckbach[1], Tineke Strouken[1], Stepan W. Koch[1], Wolfram Heimbrodt[1], Shichen Fu[2], Xiaotian Wang[2], Kyung Nam Kang[2], and Arash Rahimi-Iman[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]Department of Mechanical Engineering, Stevens Institute of Technology, Hoboken, New Jersey, 07030, USA

Two-dimensional semiconductors such as transition-metal dichalcogenides have attracted considerable attention due to their strong light-matter interaction as well as "valleytronic" properties. The valley-dependent polarization properties are of potential interest for future devices and, both, homojunctions as well as heterostructures of monolayer materials promise considerable valley-polarization degrees and valley coherence.

In this work, chemical-vapour-deposition-grown AA' and AB stacked tungsten-disulfide bilayers are investigated. The differences between AA' and AB stacked bilayers are characterized optically and attributed to the distinct interlayer coupling between k-space valleys. Our spectroscopic investigations are supported by calculations focusing on the difference in symmetry and interlayer electronic coupling for these bilayers. A comparably high valley polarization and valley coherence is found for the AB stacked case in contrast to the AA' case, which is in good agreement with the expectations.

CPP 65.2 Fri 9:45 H36

Exciton-lattice coupling in monolayer WSe2 investigated by femtosecond electron diffraction — •Shuo Dong[1], Daniela Zahn[1], Robert Schneider[2], Thomas Vasileiadis[1], Helene Seiler[1], Yingpeng Qi[1], Rudolf Bratschitsch[2], and Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institute of Physics and Center for Nanotechnology, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

Exciton-phonon coupling as the essential exciton relaxation mechanism plays a crucial role in transition metal dichalcogenides (TMDC). Besides the bright exciton dynamics, the formation of dark excitons greatly impacts the optoelectronic properties of atomically thin TMDC, which requires spin flip-scattering or phonon-assisted momentum transfer. Here, we investigate the incoherent lattice excitation associated with exciton relaxation in monolayer WSe2 by femtosecond electron diffraction. We discuss the observed structural dynamics in terms of the intra- and inter-valley exciton scattering towards the lower-lying dark states. The direct measurement of lattice motion provides important complementary insights to exciton dynamics.

CPP 65.3 Fri 10:00 H36

Towards an Atomistic Understanding of Defects in 2D Materials - Correlating Defects, Band Structure and Excitons — •Christoph Kastl[1], Roland Koch[1], Chris Chen[1], Bruno Schuler[1], Johanna Eichhorn[1], Soren Ulstrup[2], Aaron Bostwick[1], Chris Jozwiak[1], Nicholas Borys[3], Francesca Toma[1], Shaul Aloni[1], Alexander Weber-Bargioni[1], Eli Rotenberg[1], and Adam Schwartzberg[1] — [1]Lawrence Berkeley National Laboratory, Berkeley, United States — [2]Aarhus University, Denmark — [3]Montana State University, Bozeman, United States

Despite their importance, a detailed understanding of defects in 2D materials and their impact on excitonic and electronic properties is lacking. We use spatially resolved, angle resolved photoemission spectroscopy (nano-ARPES) to map the variations in band structure and defect density of monolayer WS_2 down to a resolution of 150 nm. [1] By correlating nano-ARPES with photoluminescence, we reveal the interplay between local defect density, band structure, and excitons. We compare this to atomic force and scanning tunneling microscopy, where we unambiguously identify defects at the atomic level. Surprisingly, the chalcogen vacancy is not present in as-grown monolayers, although it is commonly inferred to be the dominant point defect.[2] Instead, we find that substitutional oxygen effectively passivates chalcogen vacancies, which removes the electronic in-gap state and renders correct assignment of the defect challenging.

[1] C. Kastl et al., 2D Mater. 5, 045010, 2018. [2] arXiv:1810.02896, arXiv:1810.03364.

CPP 65.4 Fri 10:15 H36

Magnetic Anisotropic Behavior in Two-Dimensional Layered $Cr_2Ge_2Te_6$ Crystals — •Sebastian Selter[1,2], Gaël Bastien[1], Anja U. B. Wolter[1], Saicharan Aswartham[1], and Bernd Büchner[1,2] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany

$Cr_2Ge_2Te_6$ is one of the few known examples of two-dimensional layered ferromagnetic insulators. Ferromagnetic order was observed down to the bilayer, while theoretical calculations even suggest stable ferromagnetic order on the monolayer. This finding makes this compound interesting in terms of both fundamental understanding as well as for novel spintronic applications.
Thus, to entangle the physics behind possible monolayer ferromagnetism it is essential to understand the bulk magnetism which will enable us for the future applications. Here, we present a comprehensive synthesis, magnetic and thermodynamic investigation on $Cr_2Ge_2Te_6$. Bulk $Cr_2Ge_2Te_6$ becomes ferromagnetic below 64 K with the magnetic easy axis parallel to the crystallographic c-axis. A magnetic anomaly has been observed for low external fields applied perpendicular to the easy axis. An investigation of the field dependency of this anomaly hints towards a field driven nature.

CPP 65.5 Fri 10:30 H36

Nanoscale Mapping of Charge Transfer at SnS/MoS_2 2D-2D p-n Junctions Created via Low-Temperature Epitaxy — •Alex Henning[1,2], Jack N. Olding[1,3], Michael J. Moody[1], Jason Dong[1], Emily A. Weiss[3], and Lincoln J. Lauhon[1] — [1]Department of Materials Science and Engineering, Northwestern University, USA — [2]Walter Schottky Institute and Physics Department, Technische Universität München — [3]Department of Chemistry, Northwestern University, USA

Many novel two-dimensional (2D) van der Waals (vdW) heterostructures with intriguing properties for optical and electronic applications have been created by mechanical exfoliation and stacking. The ability to directly grow vdW heterostructures over large areas would create new opportunities for large-scale integration. Here, p-type tin sulfide (SnS) is grown on n-type molybdenum disulfide (MoS_2) in an atomic layer deposition (ALD) reactor at low temperatures (180 °C) to form vertical p-n 2D-2D heterojunctions (HJs). X-ray diffraction and electron backscatter diffraction establish an axiotaxial relationship between the two crystals. Kelvin probe force microscopy (KPFM) combined with a tunable illumination source is used to characterize the topography, potential landscape and photoresponse of the MoS_2/SnS HJs with a lateral resolution < 50 nm. The gained structural and electronic properties were used to optimize the parameters for the growth of electronically active SnS of controlled thickness. The built-in potential difference of 0.9 eV, measured between MoS_2 and SnS, is significantly larger than those previously reported for 2D HJs.

CPP 65.6 Fri 10:45 H36

Controlling band alignment at heterointerfaces using atomically thin Janus structures with built-in dipoles — •Simone Manti — Technical University of Denmark, Kongens Lyngby, Denmark

Recently Janus MoSSe monolayers have been synthesized by replacing S by Se on one side of MoS2. This material is an example of an atomically thin Janus structure, in which the inversion symmetry in the plane is broken leading to a finite out of plane dipole moment. Here we demonstrate that by inserting a MoSSe layer between two semiconductors, or between a semiconductor and a metal, it is possible to control the band alignment, or Schottky barrier, at the interface in a highly predictable manner. Using high-throughput density functional theory (DFT) calculations we screen for new, stable 2D Janus structures. This leads to a library of potentially synthesizable 2D materials with out-of-plane dipoles of varying strength corresponding to potential shifts between 0 and 2 eV. Our work opens new directions for rational design of band alignment at heterointerfaces.

15 min. break

CPP 65.7 Fri 11:15 H36

Theory of electron-exciton scattering in atomically thin semiconductors — Christian Fey[1], Peter Schmelcher[1], Atac Imamoglu[2], and •Richard Schmidt[3] — [1]Universität Hamburg, Germany — [2]ETH Zürich, Switzerland — [3]MPI of Quantum Optics, Garching, Germany

Excitons interacting with charge carriers in van-der-Waals materials represent a new venue to study the many-body physics of strongly interacting Bose-Fermi mixtures. In order to derive an effective low-energy model for such systems we develop an exact diagonalization approach that predicts the bound and scattering properties of electron, excitons, and trions in two-dimensional semiconductors. By solving the quantum mechanical three-body problem of interacting charge carriers we obtain binding energies of excitons and trions that are in excellent agreement with quantum Monte Carlo predictions. Importantly, in our approach also excited states are accessible. This allows us to study exotic excited trion states as well as to predict the scattering phase shifts of electrons and excitons. From these results we derive an effective low-energy model of exciton-electron scattering that can serve as an input to advanced many-body techniques. As a demonstration we study the recently observed exciton Fermi polarons, and we show that effective range corrections predicted by our model have a substantial impact on the optical absorption spectrum of charge-doped transition-metal dichalcogenides. Our approach can be applied to a plethora of many-body phenomena realizable in atomically thin semiconductors ranging from exciton lattices and localization to induced superconductivity.

CPP 65.8 Fri 11:30 H36

Computational characterization of novel 2d-materials for applications in energy and electronics — •Davide Campi[1], Thibault Sohier[1], Cedric Klinkert[2], Simran Kumari[1], Marco Gibertini[1], Nicolas Mounet[1], Mathieu Luisier[2], and Nicola Marzari[1] — [1]École polytechnique fédérale de Lausanne, Lausanne, Switzerland — [2]ETH Zurich, Zurich, Switzerland

Novel materials are crucial to future progress in information-and-communications technologies (ICT) and in energy harvesting, conversion, and storage. 2D materials provide an entire novel playground to discover novel properties and functionalities. The recent identification of many novel monolayers [1] has made available a large portfolio of materials to be explored. In this work we present an applications-oriented screenings aimed at the identification of the most promising candidates for photocatalytic water splitting, field-effect transistor channels and superconductivity.

CPP 65.9 Fri 11:45 H36

Magnetic hallmarks of viscous electron flow in graphene — •Karina A. Guerrero-Becerra[1], Francesco M. D. Pellegrino[2,3], and Marco Polini[1,4] — [1]Istituto Italiano di Tecnologia, Via Morego 30, 16163 Genova, Italy — [2]Dipartimento di Fisica e Astronomia, Università di Catania, Via S. Sofia, 64, I-95123 Catania, Italy — [3]INFN, Sez. Catania, I-95123 Catania, Italy — [4]School of Physics & Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom

Electrical transport, thermal transport, and scanning gate spectroscopy measurements have been used to identify signatures of viscous electron flow in graphene, PdCoO2, and GaAs. In this regime of transport, viscosity determines electron whirlpools in the steady-state current pattern. So far, a direct experimental observation of electron whirlpools and associated backflow is still lacking. We predict that the profile of the magnetic field generated by hydrodynamic electron flow in confined geometries displays unambiguous features linked to whirlpools and backflow near current injectors. We also show that the same profiles shed light on the nature of the boundary conditions describing friction exerted on the electron fluid by the edges of the sample. Our predictions are within reach of vector magnetometry based on nitrogen-vacancy centers in diamond, a technique that access the details of 2D spatial flow patterns in graphene [1] and combines the benefits of high spatial resolution, competitive magnetic field resolution, and operability over a wide range of temperatures.

[1] J.-P. Tetienne et. al., Sci. Adv. **3**, e1602429 (2017).

CPP 65.10 Fri 12:00 H36

Strain-induced localization of interlayer excitons in a van-der-Waals heterostructure — Malte Kremser, •Moritz Meyer, Janine Gückelhorn, Kai Müller, and Jonathan Finley — Walter Schottky Institut, Technische Universität München, München, Deutschland

The intricate potential landscape of interlayer excitons (IX) in heterobilayers (HBLs) of transition metal dichalcogenides is currently undergoing intense study. [1, 2] We show that strain can be utilized to locally modify the IX potential resulting in locally trapped states, similar to the strain-related emergence of quantum emitters in monolayer WSe2. [3, 4]

We locally strain a HBL composed of MoSe2 and WSe2 by placing it on top of lithographically defined nanopillars. The strain at the nanopillar positions creates localized states that appear as new peaks in low-temperature photoluminescence (PL) measurements, red-shifted by ~50-100 meV with respect to the IX main emission. We show that in excitation-power-dependent measurements the emission features a series of discrete peaks that suggests sequential charging of the trapping potential with multiple IXs.

[1] K. Tran et al., arXiv 1807.03771
[2] K. L. Seyler et al., arXiv 1809.04562
[3] A. Branny et al., Nat. Commun. 8, 15053 (2017)
[4] C. Palacios-Berraquero et al., Nat. Commun. 8, 15093 (2017)

CPP 65.11 Fri 12:15 H36

Extreme Ultraviolet Core-Exciton Dynamics in Two-dimensional Molybdenum Disulfide — •Michael Zürch[1,8], Hung-Tzu Chang[1], Alexander Guggenmos[1], Diana Y. Qiu[2,3], Romain Geneaux[1], Yen-Chang Chen[4,5], Xuan Wei[5], Chang-Ming Jiang[6,7], Yufeng Liang[4], Felipe H da Jornada[2,3], Adam Schwartzberg[4], David Prendergast[4], Vincent C. Tung[5], Steven G. Louie[2,3], Daniel M. Neumark[1,6], and Stephen R. Leone[1,2,6] — [1]Department of Chemistry, University of California, Berkeley, USA — [2]Department of Physics, University of California, Berkeley, USA — [3]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA — [4]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, USA — [5]School of Engineering, University of California, Merced, USA — [6]Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA — [7]Joint Center of Artificial Photosynthesis, LBNL, Berkeley, USA — [8]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Novel tightly-bound core-excitons triggered by an XUV attosecond pulse are observed in two-dimensional transition-metal dichalcogenide molybdenum disulfide. State-of-the-art theory calculations confirm the observed features. The dynamics observed in the core-exciton states between the molybdenum 4p and 4d states indicate coherences, and population transfer between different states. The observation of strongly enhanced long-lived core excitons in two-dimensional semiconductors paves the way for further exploration into the properties of core excitons in two-dimensional materials and potential application of these.

CPP 65.12 Fri 12:30 H36

One-Nanometer-Thin Carbon Nanomembranes: Combining High Water Permeance with High Selectivity — •Yang Yang, Petr Dementyev, Niklas Biere, Daniel Emmrich, Patrick Stohmann, Riko Korzetz, Xianghui Zhang, André Beyer, Sascha Koch, Dario Anselmetti, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Membrane-based separation provides an energy-efficient technology in producing clean water. Recent nanotechnology breakthroughs have led to the emergence of 2D membranes which promise minimal transport resistance and thus exceedingly high molecular flow rates. Carbon nanomembranes (CNMs) are a special class of 2D materials made by crosslinking of self-assembled monolayers. In this work, we will present the rapid and selective water permeation through a 1.2-nm thin CNM fabricated from terphenylthiol (TPT) precursors [1]. TPT CNMs consist of sub-nanometer channels with a high areal density of $10^{18}\,m^{-2}$. The membrane can block the passage of most gases and liquids, while permitting water and helium to pass through. In particular, water transits with a remarkably high permeance of 1.1×10^{-4} mol $m^{-2}\,s^{-1}\,Pa^{-1}$, 2,500 times faster than helium. The rapid water flow is ascribed to a hydrogen-bonded cooperative transport inside the CNM channels.

Reference

[1] Y. Yang, *et al*. Rapid Water Permeation Through Carbon Nanomembranes with Sub-Nanometer Channels. *ACS Nano* 2018, 12, 4695-4701.

CPP 65.13 Fri 12:45 H36

Photoactive molecular nanosheets with 1 nm thickness

— •Maria Küllmer[1], Felix Herrmann-Westendorf[1,3], Stefan Götz[2], Christof Neumann[1], Patrick Endres[2], Andreas Winter[2], Ulrich Sigmar Schubert[2,4], Benjamin Dietzek[1,3,4], and Andrey Turchanin[1,4] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Institute of Organic Chemistry and Makromolecular Chemistry (IOMC), Friedrich Schiller University Jena, 07743 Jena — [3]Leibniz Institute of Photonic Technology e. V., 07745 Jena — [4]Center for Energy and Environmental Chemistry Jena (CEEC Jena), 07743 Jena

Artificial photocatalytic systems play an important role in the development of novel energy sources. Functional incorporation of molecular catalysts into two-dimensional (2D) soft matter matrixes is a prerequisite towards the realization of the artificial leaf systems. Here we present 1 nm thick photoactive molecular nanosheets - Carbon Nanomembranes (CNMs) - generated by electron irradiation induced crosslinking of self-assembled photocatalytic ruthenium-(II)-complexes on gold substrates. We characterize the chemical and structural properties of these molecular 2D systems using high-resolution X-ray photoelectron and surface enhanced Raman spectroscopy in combination with atomic force and scanning electron microscopy. We employ photothermal deflection spectroscopy to characterize the adsorption band of the formed free-standing photoactive CNMs and to compare it with the characteristics of the pristine ruthenium-(II)-complexes