CPP 83: 2D Materials (Symposium and Joint Session with HL and O): Session III (joint session DS/CPP/HL)

Time: Friday 9:30–12:30 Location: H 2032

Invited Talk CPP 83.1 Fri 9:30 H 2032

Tunable Electronic Structures, Magnetism, and Axis-Dependent Conduction Polarity in Ge and Sn-based 2D Materials — •Joshua Goldberger — The Ohio State University, Columbus, OH USA

Here, we will discuss recent developments in the synthesis, properties, and applications of two classes of Ge- and Sn-based 2D materials; the ligand-functionalized Ge/Sn graphane analogues, and the exfoliatable van der Waals Zintl phases. First, the Ge/Sn graphane analogues have generated much excitement as their electronic structures are predicted to range from trivial insulators, to semiconductors with tunable gaps, to semimetallic, to topological insulators, depending on the substrate, chemical functionalization and strain. Through the synthesis and characterization of a large family of ligand-functionalized germananes, we will show how the electronic structure can be manipulated via surface chemistry. Second, we will highlight a new family of chemically and thermally robust exfoliatable 2D materials having a stoichiometry of ASn2Pn2, where A is a cation, and Pn is a pnictogen. This class of materials can be designed to exhibit a broad range of phenomena including the topological insulating compound, SrSn2As2, as well as the magnetic compound, EuSn2As2. Also, we will show that NaSn2As2 simultaneously exhibits opposite sign conduction polarities along its in-plane and cross-plane axes. Using a variety of advanced transport measurements we establish the band structure origins of this behavior. Together, these materials show how the inherent anisotropy in 2D materials can be rationally tailored to give rise to new phenomena.

CPP 83.2 Fri 10:00 H 2032

Chemical and optical properties of transition metal dichalcogenide monolayers at the nanometer and subnanometer scale — •Luiz Tizei[1], Alberto Zobelli[1], Ching-Hwa Ho[2], Kazu Suenaga[3], Alexandre Gloter[1], Mathieu Kociak[1], and Odile Stéphan[1] — [1]Laboratoire de Physique des Solides, University of Paris-Sud, CNRS, Orsay, France — [2]National Taiwan University of Science and Technology, Taipei, Taiwan — [3]AIST, Tsukuba, Ibaraki, Japan

Defects and interface play an important role in material properties. Therefore, their characterization at the nanometer scale is crucial. Here, core-loss EELS and high angle annular dark field imaging have been used to identify single Cr atoms in WSe_2 monolayers. These atoms are always located at the metal site (W) with a 3+ formal valence, as deduced from EELS fine structure comparison with known references and X-ray photoelectron spectroscopy (XPS). Furthermore, Cr atoms are observed systematically close to single our double Se vacancies, indicating a possible electron doping of the system. Moreover, semiconducting 2H phase TMD monolayers present spin-split valence and conduction bands due to spin-orbit coupling. These two near band edge states are separated by from a few tens to a few hundred meV and can be measured by EELS with high spatial resolution. As an example, we will show measurements of the near band edge losses as a function of position across an interface between two TMDs. Results will be compared to calculated loss functions, tacking into account the materials' dielectric function.

CPP 83.3 Fri 10:15 H 2032

Excitonic Phonon Sidebands in Monolayer Transition Metal Dichalcogenides — •Dominik Christiansen[1], Malte Selig[1], Gunnar Berghäuser[2], Robert Schmidt[3], Iris Niehues[3], Robert Schneider[3], Ashish Arora[3], Steffen Michaelis de Vasconcellos[3], Rudolf Bratschitsch[3], Ermin Malic[2], and Andreas Knorr[1] — [1]Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, Gothenburg, Sweden — [3]Physikalisches Institut und Zentrum für Nanotechnologie, Universität Münster, 48149 Münster, Germany

Monolayers of transition metal dichalcogenides (TMDs) show an extraordinarily strong Coulomb interaction, leading to the formation of tightly bound excitons. Because of a complex quasi-particle band structure, TMDs possess a variety of bright sates (addressable by light) and dark states (addressable by phonons). Here, we present a joint experiment-theory study on the influence of exciton-radiative and exciton-phonon interaction on the absorption line shape of different monolayer TMD materials. Solving the TMD Bloch equations in the quantum kinetic limit, we predict the appearance of spectrally asymmetric phonon-induced sidebands that are accompanied by a pronounced polaron-red shift. We analyze the influence of the interplay of phonon emission/absorption processes and dark intra- and intervalley excitonic states on the asymmetry of the absorption line shape.

D. Christiansen, et. al, Phys. Rev. Lett. 119, 187402 (2017)

CPP 83.4 Fri 10:30 H 2032

Lifetime of Valley Excitons in Monolayer Transition Metal Dichalcogenides — •Malte Selig[1], Samuel Brem[2], Florian Katsch[1], Gunnar Berghäuser[2], Ermin Malic[2], and Andreas Knorr[1] — [1]Nichtlineare Optik und Quantenelektronik von Halbleitern, Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, Gothenburg, Sweden

In monolayers of transition metal dichalcogenides, weak screening leads to the formation tightly bound excitons which dominate the optical properties of these ultrathin materials. A pronounced circular dichroism leads to a spin and valley selective excitation of excitons at the corners of the hexagonal Brillouin zone. A microscopic understanding of the lifetime of such optically injected spins is of crucial interest for future technological applications. Here, based on a Heisenberg of motion formalism for excitons, we perform microscopic momentum and spin resolved computations to investigate the impact of exciton phonon coupling and intervalley exchange coupling on the valley lifetime of excitons. In our analysis, we also include recently discussed indirect dark excitons [1,2]. In the absence of low lying dark states we find valley lifetimes below 1 ps, which increases by orders of magnitude if the material is indirect.

[1] M. Selig et al., Nat. Commun. 7, 13279 (2016)
[2] M. Selig et al., arXiv:1703.03317 (2017)

CPP 83.5 Fri 10:45 H 2032

Interface sensitive structure determination of silicon nano-ribbons on Gold surfaces — •Peter Roese[1,2], Philipp Espeter[1,2], Karim Shamout[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1, Technische Universität Dortmund, Germany — [2]DELTA, Technische Universität Dortmund, Germany

In the last years there has been much progress in the growth and analysis of 2D-materials beyond graphene on metallic surfaces. Especially, silicon based two-dimensional silicene and one-dimensional silicon nano-ribbons came into scientific focus due to their promising electronic properties. Beside the exact knowledge of the fascinating electronic and chemical properties of such systems, the structural information is of great interest for precise DFT calculations. In this context the interaction between the silicon nano-ribbons and the substrate plays an important role. Techniques like STM or LEED provide information about the electronic structure of such systems but neither chemical information about the atomic bonds nor information about the interface. Photoelectron spectroscopy and diffraction easily provide information about atomic bonds and the interface between silicon nano-ribbons and the substrate, recently shown by Espeter et al [8]. The structure of silicon nano-ribbons on Ag(110) has recently been resolved whereas their exact structure on Au(110) and the effect of the interface needs to be analyzed in detail. Based on previous works, we present first photoelectron diffraction results of silicon nano-ribbons on Au(110).

15 min. break.

CPP 83.6 Fri 11:15 H 2032

Disclosing the nature of excitons in van der Waals materials: The role of layer stacking in hexagonal boron nitride — •Wahib Aggoune[1,2], Caterina Cocchi[2,3], Dmitrii Nabok[2,3], Karim Rezouali[1], Mohamed Akli Belkhir[1], and Claudia Draxl[2,3] — [1]Laboratoire de Physique Théorique, Faculté des Sciences Exactes, Université de Bejaia, 06000 Bejaia, Algeria — [2]Institut fur Physik and IRIS Adlershof, Humboldt-Universitat zu

Berlin, Berlin, Germany — [3]European Theoretical Spectroscopic Facility (ETSF)

With the example of bulk hexagonal boron-nitride, a prototypical van der Waals (vdW) crystal, we demonstrate that the electronic and optical properties of these materials can be tuned by layer patterning. By modifying the stacking, energy, intensity, and character of the electron-hole (e-h) pairs can be selectively modulated. Depending on the specific layer arrangement, lowest-energy excitons are localized within a single layer or delocalized in the three-dimensional space. Only in specific stackings charge-transfer e-h pairs appear above the absorption onset, triggered by the spatial distribution of the electronic states involved. Our results, obtained within a first-principles many-body framework, provide all the ingredients to identify, predict, and tailor the character of the e-h pairs in vdW materials.

CPP 83.7 Fri 11:30 H 2032

Evidence for low-dimensional charge transport in carbon nitride polymers — •Christoph Merschjann — Helmholtz-Zentrum-Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

Carbon nitride (CN) polymers have gained much interest in recent years due to their potential application as both dark- and photocatalysts for various renewable-energy tasks, including water-splitting and CO_2 reduction, and others. Given their layered, van-der-Waals bound structure, these materials resemble graphite, and are hence often called "graphitic carbon nitrides" (g-C_3N_4). The main technical advantage of CNs is the abundance of their constituents (C, N, and H) and the absence of precious metals. However, compared to metal-based catalysts, the activity of CN materials is still rather low, a fact that has been largely attributed to their low conductivity. Recently, we found evidence that this low conductivity is due to polaronic hopping motions of photoexcited electrons and holes, which predominantly move vertical to the graphitic planes of the material. Backed-up by very recent transient-spectroscopy studies, we will discuss the validity of such a low-dimensional transport scenario, and its consequences for applications in catalysis as well as in organic electronics in general.

CPP 83.8 Fri 11:45 H 2032

Deterministic Positioning of Single-Photon Emitters in Monolayer WSe_2 on the Nanoscale — •Johannes Kern[1], Iris Niehues[1], Philipp Tonndorf[1], Robert Schmidt[1], Daniel Wigger[2], Robert Schneider[1], Torsten Stiehm[1], Steffen Michaelis de Vasconcellos[1], Doris E. Reiter[2], Tilman Kuhn[2], and Rudolf Bratschitsch[1] — [1]Institute of Physics and Center for Nanotechnology, University of Münster, Germany — [2]Institute of Solid State Theory, University of Münster, Germany

Single-photon emitters are an important building block for photonic quantum technology. Here, we deterministically position single-photon emitters in monolayer WSe_2 on the nanoscale [1]. The atomically thin semiconductor is placed on top of a gapped single-crystalline gold rod which results in a folding of the monolayer around the metal nanostructure. At the gap position, local strain is induced in the atomically thin semiconductor. Excitons localize there and radiatively decay via single-photon emission.

[1] J. Kern et al., "Nanoscale positioning of single-photon emitters in atomically thin WSe2", Adv. Mater. 28, 7101-7105, (2016).

CPP 83.9 Fri 12:00 H 2032

Pulsed Laser Deposition of Monolayer WSe_2 — •Avaise Mohammed[1], Hiroyuki Nakamura[1], Peter Wochner[1], Shyjumon Ibrahimkutty[1], Armin Schulz[1], Kathrin Müller[1], Krystian Nowakowski[2], Keita Matsuda[3], Johannes Geurs[1], Yijin Zhang[1], Mona Stadler[4], Kenji Watanabe[5], Takashi Taniguchi[5], Benjamin Stuhlhofer[1], Georg Cristiani[1], Gennady Logvenov[1], Michael Jetter[4], Peter Michler[4], Jurgen Smet[1], Ulrich Starke[1], and Hidenori Takagi[1,6] — [1]MPI-FKF — [2]University of Twente — [3]Nagoya University — [4]IHFG, University of Stuttgart — [5]NIMS — [6]IFMQ, University of Stuttgart

Ultrathin WSe_2 films were deposited using a custom built hybrid-Pulsed Laser Deposition (PLD) system on different substrates. Raman spectroscopy and atomic force microscopy were used to identify the monolayer (ML) WSe_2. Synchrotron based grazing incidence X-ray diffraction revealed WSe_2 films to have a compressive strain on Al_2O_3 r-cut substrates. Angle resolved photoelectron spectroscopy confirmed the valance band structure of ML WSe_2 on epitaxial graphene with a clear spin splitting of 480 meV. Photoluminescence signal was identified from ML WSe_2 deposited on hexagonal BN. The results give evidence for PLD to be an excellent approach for the growth of monolayer transition metal chalcogenides.

CPP 83.10 Fri 12:15 H 2032

Gate-dependent spin dynamics of dark trion states in monolayer WSe_2 — •Manfred Ersfeld, Frank Volmer, Maximilian Heithoff, Christopher Franzen, Christoph Stampfer, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

We explore the spin dynamics in WSe_2 monolayers by time-resolved Kerr rotation measurements. The longest spin lifetimes of up to 150 ns are observed at 5 K when resonantly pumping into charged exciton states (trions). We explain these long spin lifetimes by the formation of dark trion states which exhibit equal recombination lifetimes independently measured by time-resolved reflectivity [1]. We show that the spin lifetimes of the dark trion states strongly depend on the chemical potential which we tune by applying a gate voltage to the WSe_2 flake through a SiO_2/Si^{++} substrate. The formation of the dark trion states require intervalley scattering driven by short range scattering centres. Additional photoluminescence measurements indicate that this short range scattering is caused by localized states and gets strongly diminished with increasing temperature which may also be relevant for the overall strong decrease of both the spin amplitude and the spin lifetime of the dark trion states with increasing temperature.

[1] F. Volmer et al., Phys. Rev. B 95, 235408 (2017)