HL 34: 2D Materials V (joint session HL/CPP)

Time: Thursday 9:30–12:00 Location: POT 81

HL 34.1 Thu 9:30 POT 81

Negative differential resistance with ultra-high peak-to-valley current ratio in tunnel diodes based on two-dimensional cold metals — •Ersoy Sasioglu and Ingrid Mertig — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, 06120 Halle (Saale)

The negative differential resistance (NDR) effect is of great interest for future memory and logic circuit applications. We propose a novel semiconductor-free NDR tunnel diode concept with ultra-high peak-to-valley current ratio (PVCR) [1]. Our proposed NDR diode consists of two cold metal electrodes separated by a thin insulating tunnel barrier. The NDR effect stems from the unique electronic band structure of the cold metal electrodes, i.e., the width of the isolated metallic bands around the Fermi level as well as the energy gaps separating higher- and lower-lying bands determine the current-voltage characteristics and PVCR value of the tunnel diode. By proper choice of the cold metal electrodes either Λ-type or N-type NDR effect can be obtained. We employ the nonequilibrium Green's function method combined with density functional theory to demonstrate the NDR characteristics of the proposed diode based on two-dimensional NbS_2/h-BN/NbS_2 vertical and AlI_2/MgI_2/AlI_2 planar heterojunctions. For the lateral tunnel diode, we obtain a Λ-type NDR effect with an ultra-high PVCR value of 10^{16} at room temperature, while the vertical tunnel diode exhibits a conventional N-type NDR effect with a smaller PVCR value of about 10^4. The proposed concept provides a semiconductor-free solution for NDR devices to achieve desired I-V characteristics.

[1] Ersoy Şaşıoğlu and Ingrid Mertig, arXiv:2207.02593 (2022).

HL 34.2 Thu 9:45 POT 81

Electrical contact engineering on 2D material through ion implantation and flash lamp annealing — •kaiman lin[1,2], yi li[2], manfred helm[2], shengqiang zhou[2], yaping dan[1], and slawomir prucnal[2] — [1]University of Michigan-Shanghai Jiao Tong University Joint Institute, Shanghai Jiao Tong University, 20024 Shanghai, P. R. China — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

In recent years, 2D material-based nanodevices have been extensively studied and exhibit highly competitive performance compared with conventional bulk semiconductors. Before they can be fully integrated with existing Si-based technology or offer new platform for novel nanoelectronics, some challenges must be solved. One of the key challenges in 2D devices is the large Schottky barrier at the 2D/metal interface, which limits the charge carrier injection from metal to 2D channel. In this paper, we propose a novel method, which exploits the top metal electrode as the capping layer during the ion implantation process, followed by ms-range flash lamp annealing to repair the defects caused by ion implantation and to activate dopants. Our approach allows to realize effective doping at the interface between multilayer 2D materials and metal electrodes and simultaneously minimize the defect concentration created during the ion implantation process. As a result, the ohmic contact between 2D material and metal electrodes will be realized.

HL 34.3 Thu 10:00 POT 81

Impact of free carriers on exciton and trion diffusion in monolayer WSe2 — •Marzia Cuccu[1], Koloman Wagner[1], Zakhar A. Iakovlev[2], Jonas D. Ziegler[1], Takashi Taniguchi[3], Kenji Watanabe[3], Mikhail M. Glazov[2], and Alexey Chernikov[1] — [1]TU Dresden, Dresden, Germany — [2]St. Petersburg, Russia — [3]National Institute for Materials Science, Tsukuba, Japan

In monolayer transition metal dichalcogenides excitons are tightly bound, mobile at room and cryogenic temperatures, and interact strongly with free charge carriers. However, the role of the exciton-electron interaction in the context of exciton propagation remains unclear. Here, we address this question by demonstrating diffusion of excitons in hBN-encapsulated WSe2 in the presence of a continuously tunable Fermi sea. Using ultrafast microscopy, we reveal a non-monotonic dependence of the exciton diffusion coefficient on the charge carrier density in both electron- and hole-doped regimes. We identify distinct regimes of elastic scattering and quasiparticle formation determining exciton diffusion and highlight the importance of treating exciton-electron scattering in the presence of additional energy and momentum dissipation via phonons. We further show that trions remain mobile even at low temperatures down to 5 K, with an effective trion mobility up to 3000 cm2/(Vs).

HL 34.4 Thu 10:15 POT 81

Electrical Characterization of Thin $ZrSe_3$ Films — •Lars Thole[1], Christopher Belke[1], Sonja Locmelis[2], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

Two dimensional materials have been of great interest in the past years, because of their huge potential for new applications [1]. While graphene has been extensively researched, a lot of other materials have emerged. One of the most notable groups are the transition metal chalcogenides because of their variety of different compounds. Among these the lesser known transition metal trichalcogenides show unique properties [2].

Here, we have researched the transition metal trichalcogenide $ZrSe_3$ [3]. Its bulk material was produced by a chemical vapor transport method and was then exfoliated to obtain thin films. Electrical measurements show a band gap of 0.6 eV which increases for thinner samples. The material is shown to be an n-type semiconductor by transistor measurements and a mean free path of about 103 nm was determined by looking at different samples with varying thicknesses.

[1] A. K. Geim, I. V. Grigorieva, Nature, 499, 419-425 (2013).
[2] J. O. Island et al., 2D Materials, 4, 0220033 (2017).
[3] L. Thole et al., ACS Omega, 7, 39913 (2022).

HL 34.5 Thu 10:30 POT 81

Electrically active deep defects in 2D vdW semiconductors — •Michele Bissolo[1], Rongxin Li[1], Masako Ogura[2], Svitlana Polesya[2], Hubert Ebert[2], Eugenio Zallo[1], Gregor Koblmüller[1], and Jonathan J. Finley[1] — [1]Walter Schottky Institute and TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany — [2]Department of Chemistry/Phys. Chemistry, LMU Munich, Butenandtstrasse 11, 81377 Munich, Germany

Mid-gap defect states in semiconductors can both potentially degrade the performance of (opto)electronic devices and simultaneously act as a platform for technologies such as (photo)catalysis and quantum computing. Characterizing the electrically active mid-gap defects in the emerging class of 2D van-der-Waals materials is thus a necessary step in the development of future 2D-based devices. Here, we employ Deep Level Transient Spectroscopy (DLTS) techniques to directly probe deep defects in transition metal dichalcogenides (TMDCs) and group-III monochalcogenides (III-MCs), which have recently gained traction in "more-than-Moore", low-power and renewable energy device applications. Unlike transmission electron or scanning tunneling microscopies, DLTS is both a non-destructive and bulk sensitive technique that provides multiple information on the electronically active defect states, such as concentration, energy and capture cross section. DLTS spectra are collected from few-layer MoS_2, $MoSe_2$ and GaSe Schottky diodes in the 10-300 K temperature range with 10 mK stability, and the properties and role of the observed defects are discussed.

15 min. break

HL 34.6 Thu 11:00 POT 81

Ionic based gate control of insulator-to-metal phase transitions on ZrS_2 — •Jose Guimaraes[1,2], Dorsa Fartab[1], Marcus Schmidt[1], and Haijing Zhang[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS, UK

The possibility of tuning the properties of solids, such as their carrier density, allows for the amplification of their potential: In the context of 2D materials, ionic liquid gating provides a highly efficient doping alternative to traditional chemical doping.

Transitional metal dichalcogenides (TMDCs) have emerged as a potential 2D replacement for silicon in many technological applications, however their carrier mobility needs to be vastly increased. Ionic liquid gating enables carrier concentrations of the order of 10^{14} carriers per cm^2 in certain TMDCs, moreover, it allows for the emergence of unique physical phenomena, such as ambipolar behaviour. To realize transistor applications, materials that can be easily switched between p-type and n-type by applying an electric field are essential to minimize circuit size.

Here, an overview of the ionic liquid gating technique is given, including device fabrication and characterization methods, focusing on the TMDCs: ZrS_2 and $ZrSe_2$. Being $ZrSe_2$ an oxygen sensitive material, a method of estimating its thickness by its optical image is discussed. Furthermore, experimental efforts reporting ambipolar behaviour in ZrS_2 for the first time are presented.

HL 34.7 Thu 11:15 POT 81

Lattice reconstruction in twisted transition metal dichalcogenide heterobilayers — •Wei Li, Thomas Brumme, and Thomas Heine — TU Dresden, Dresden, Germany

Twisted heterostructures of 2D crystals have resulted in a series of high-impact contributions to condensed matter physics, most prominently flat bands and superconductivity in twisted bilayer graphene. But also two-dimensional crystals beyond graphene, such as transition metal dichalcogenides, show strong proximity effects that are affected by twisting. Here, we systematically investigate the structural impact of twist angles on transition metal dichalcogenide van der Waals heterobilayers consisting of MoS_2, WS_2, $MoSe_2$ and WSe_2 monolayers. We find that the significant lattice reconstruction involving in- and out-of-plane displacements strongly depends on the twist angle: from a continuous variation of local stacking alignment at large twist angles to a soliton-domain structure at small twist angles. Especially, starting from either 2H or 3R stacking, two different critical twist angles exist, above which the two constituting layers show dramatically asymmetrical corrugation, in contrast to the symmetry-preserving out-of-plane deformation in twisted homobilayers. We reveal that the development of either the corrugation or the soliton-domain results from the competition between strain energy cost and van der Waals energy gain. Our calculations show that van der Waals heterobilayers develop, besides the well-investigated moiré structures, also systems with large areas of special local stackings arranged in a superlattice, suggesting intriguing electronic properties of these systems.

HL 34.8 Thu 11:30 POT 81

Pump Probe Signatures of Interlayer Excitons in TMDC Heterostructures — •Henry Mittenzwey[1], Manuel Katzer[1], Benjamin Kaiser[2], Veronica Policht[3], Oleg Dogadov[3], Stefano Dal Conte[3], Giulio Cerullo[3], Andreas Knorr[1], and Malte Selig[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Zuse Institute Berlin, Takustraße 7, 14195 Berlin, Germany — [3]Dipartimento di Fisica, Politecnico di Milano, I-20133 Milano, Italy

TMDC heterobilayers are promising candidates for novel optoelectronic applications, since they exhibit long-lived excitonic states with spatially separated electrons and holes located in different layers. The relaxation dynamics of these interlayer excitons and their interplay with intralayer excitons are still under investigation.

Here, we present a microscopic description for the phonon and tunneling induced formation and relaxation of intra- and interlayer excitons in a $MoSe_2/WSe_2$ stack. Based on the microscopic dynamics we calculate the pump probe signal for intra- and interlayer transition and their population dynamics including hot exciton bottleneck effects and unbound interlayer occupations.

HL 34.9 Thu 11:45 POT 81

Microscopic picture of interlayer exciton-phonon coupling — Muralidhar Nalabothula, Ludger Wirtz, and •Sven Reichardt — University of Luxembourg, Luxembourg

Excitons play a key role for opto-electronic applications of 2D heterostructures. They also can strongly couple to phonons as evidenced by their imprint on resonant Raman scattering intensities [1,2]. In 2D heterostructures, this sort of strong coupling and its signature Raman scattering offers an ideal setting to learn about exciton-phonon coupling both within and across material layers. Here we focus on the example of monolayer WSe2 and hBN. Its Raman spectrum features the norminally silent out-of-plane optical phonon mode of hBN that becomes active due to symmetry breaking and - most curiously - very strongly enhanced due to resonant exciton-phonon scattering [1]. While the resonant scattering pathways have been identified as involving excitons in WSe2 that couple to the phonons in hBN [1], a microscopic understanding of this interlayer exciton-phonon coupling is still missing. We provide such understanding using the state-of-the-art method for the computation for resonant Raman scattering intensities [2,3], which allows a detailed atomistic and quantum mechanical dissection of the Raman scattering process. Supplemented by a classical picture, our work sheds light on the microscopic mechanism behind exciton-phonon coupling in 2D heterostructures.

[1] C. Jin, et al. Nat. Phys., 13, 127-131, (2017).
[2] S. Reichardt and L. Wirtz. Sci. Adv. 6, eabb5915, (2020).
[3] S. Reichardt and L. Wirtz. Phys. Rev. B 99, 174312, (2019).