

DS 2: 2D Materials: Session I (joint session DS/ CPP/HL)

Time: Monday 9:30–13:15

Location: H 2032

DS 2.1 Mon 9:30 H 2032

Graphene nanoribbon: electronic band structure, doping and Raman fingerprints — ●BORIS SENKOVSKIY¹, DMITRY USACHOV², ALEXANDER FEDOROV^{2,3}, GIANNI PROFETA⁴, DANNY HABERER⁵, FELIX FISCHER⁵, and ALEXANDER GRÜNEIS¹ — ¹II. Institute of Physics, University of Cologne, Cologne, Germany — ²St. Petersburg State University, St. Petersburg, Russia — ³IFW-Dresden, Dresden, Germany — ⁴Department of Physical and Chemical Sciences and SPIN-CNR, University of L'Aquila, Coppito, Italy — ⁵Department of Chemistry, University of California at Berkeley, Berkeley, USA

We present the state-of-the-art studies of atomically precise graphene nanoribbons (GNRs) synthesized using on-surface assisted molecular assembly. Using angle-resolved photoemission spectroscopy (ARPES), we obtain the band structure of pristine and boron-doped armchair GNRs of $N=7$ carbon atoms width. ARPES maps in the full 2D momentum space visualize each sub-band of quasi-1D GNRs and allow to extract effective masses, charge carrier velocities and sub-band energy offsets. Vibration properties of GNRs are probed in-situ by ultra-high vacuum Raman setup. We show how the periodically incorporated boron atoms affect the band structure and the Raman-active modes of GNRs. Particularly, in doped nanoribbons the effective mass of charge carriers is ~ 2 times smaller and the peculiar Raman modes are red-shifted and doubled regarding to the pristine system.

[1] Senkovskiy et al. Adv. Electron. Mater. 2017.

[2] Senkovskiy et al. Nano Lett., 2017.

[3] Senkovskiy et al. Phys. Status Solidi RRL, 2017.

DS 2.2 Mon 9:45 H 2032

Valley spin lifetimes reaching 100 ns in monolayer MoSe₂ at room temperature — ●MAXIMILIAN HEITHOFF, MANFRED ERSFELD, FRANK VOLMER, ROBIN DE WINTER, CHRISTOPH STAMPFER, and BERND BESCHOTEN — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

We present time-resolved Kerr-rotation measurements on a monolayer of MoSe₂ revealing spin lifetimes up to 100 ns at room temperature. This extraordinary long-lived spin signal only weakly depends on temperature between 60 K and 300 K. At lower temperatures, it gets masked by an additional spin signal with significantly larger amplitude but shorter spin lifetimes reaching 8 ns. The latter spin signal exhibits a Kerr resonance which coincides with the photoluminescence spectrum from neutral and charged excitons showing that the spin dynamics at low temperatures are dominated by excitonic effects. In contrast, the long-lived spin signal at higher temperatures shows no resonance in the energy regime of the excitons. The absence of such resonance combined with the long spin lifetimes at room temperature is expected if the spin dynamics at elevated temperatures are not dominated by excitonic effects but by a polarization of resident holes, which is protected even at room temperature due to the large spin splitting in the valence bands of transition metal dichalcogenides.

DS 2.3 Mon 10:00 H 2032

Ultra-high vacuum Raman spectroscopy of Cs doped monolayer graphene — ●MARTIN HELL, BORIS SENKOVSKIY, JOSHUA HALL, THOMAS MICHELY, and ALEXANDER GRÜNEIS — II. Physikalisches Institut, Universität zu Köln

We show that ultra-high vacuum (UHV) Raman spectroscopy is a valuable tool for in-situ characterization of epitaxial graphene on Ir(111) regarding strain, defects and doping level. We study the Cs doping induced changes in the Raman spectrum of epitaxial monolayer graphene for 2×2 and $\sqrt{3} \times \sqrt{3}$ Cs adsorption geometries for exciting laser energies in a wide range (325nm to 633nm). The combined effects of lattice expansion and dynamic effects lead to characteristic changes in the Raman spectrum that allow us to identify the charge transfer and the electron-phonon coupling strength from the position, width and asymmetry of the G band Raman line. The electronic and structural characterization of Cs doped graphene is complemented by angle-resolved photoemission measurements and scanning tunneling microscopy on identically prepared samples. The high energy resolution of Raman (~ 1 wavenumber) allows for a precise determination of temperature induced strain of epitaxial graphene. Finally, we will show new results regarding the UHV Raman and luminescence characterization of transition metal dichalcogenides grown on graphene/Ir(111).

DS 2.4 Mon 10:15 H 2032

Raman spectroscopy of misfit layer compound nanotubes from CrS₂ and TaS₂ — ●FELIX KAMPMANN^{1,2}, DALIT STOLOVAS³, LEELA S. PANCHAKARLA³, GAL RADOVSKY³, CHRISTIAN THOMSEN², RESHEF TENNE³, and JANINA MAULTZSCH² — ¹Institut für Festkörperphysik, TU Berlin, Berlin, Germany — ²Institut für Physik der Kondensierten Materie, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — ³Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel

Misfit layer compounds (MLC) offer an interesting approach towards synthesis of novel one-dimensional nanostructures and two-dimensional materials. Understanding their structure and their physical properties has been subject to intense scientific research. The MLCs described by the formula $MX-TX_2$ consist of a transition metal dichalcogenide (TMD) layer TX_2 and an intercalation layer MX with distorted rock-salt structure. Here M denotes a metal, X is one of the elements S or Se, and T is of the group of transition metals.

In our study the TMD layer CrS₂ or TaS₂ is intercalated by either LaS-, CeS- or GdS- layers. Upon formation of the MLC charge transfer between the sublayers and deformation of the intercalation layer stabilize the otherwise metastable CrS₂. Due to the misfit between the sublayers in at least one direction and the seaming of dangling bonds at the rim atoms, the synthesis of nanotubes and -scrolls is favored. We investigate the vibrational properties of MLC nanotubes via Raman spectroscopy and discuss the results regarding previously published TEM methods.

DS 2.5 Mon 10:30 H 2032

Photoluminescence study of MoS₂ monolayers integrated with photonic nanostructures — ●RAJESHKUMAR MUPPARAPU¹, TOBIAS BUCHER¹, ANTONY GEORGE², FRANK SETZPFANDT¹, THOMAS PERTSCH¹, ANDREY TURCHANIN², and ISABELLE STAUDE¹ — ¹Institute of Applied Physics, Abbe Center of Photonics, Friedrich Schiller University Jena, 07745 Jena, Germany — ²Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany

Interaction of light with MoS₂ monolayers can be enhanced by integrating them with resonant nanostructures [1], and such interaction allows to manipulate their photoluminescence (PL) directionality and polarization. Here, we investigated the PL properties of MoS₂ monolayers integrated with resonant Silicon nanostructures [2] to explore the behavior of PL and valley polarization. Experiments performed on MoS₂-nanostructures reveal a significant PL enhancement [3], dominantly due to the local strain rather than Purcell enhancement. We further studied the valley polarization of MoS₂ flakes under different locally modified environments.

References:

[1]. S. Butun, *et al.*, Nano Lett., 2015, 15, 2700-2704.

[2]. M. Decker, I. Staude, J. Opt. 18, 103001 (2016).

[3]. T. Bucher, *et al.*, CLEO/Europe-EQEC 2017, Munich, EI-4.5, (2017).

DS 2.6 Mon 10:45 H 2032

luminescence at defects in h-BN : excitons at stacking faults and single photon emitters — ●ALBERTO ZOBELLI, ROMAIN BOURRELLIER, SOPHIE MEURET, MICHELE AMATO, ODILE STÉPHAN, LUIZ TIZEI, and MATHIEU KOČIAK — Laboratoire de Physique des Solides, University of Paris-Sud, CNRS, Orsay, France

h-BN is a promising material for optical application due to a strong exciton in the far UV and bright and stable defect emissions. Here we investigate the spatial localization at the nanometric scale of defects lines in this rich emission spectrum by employing an original cathodoluminescence system (nano-CL) integrated within a scanning transmission electron microscope. We show that high energy emissions are related to crystal folds leading to local changes of the layer stacking order which promote additional excitons. Furthermore, middle band gap emissions present a high spatial localization (~ 80 nm) and a typical zero-phonon line plus phonon replica spectroscopic signature, indicating a point defect origin. Finally, by combining our nano-CL system with an Hanbury Brown and Twiss (HBT) interferometer we identify a new bright and stable single photon emitter in the far UV.

DS 2.7 Mon 11:00 H 2032

Density-functional perturbation theory for gated 2D heterostructures — ●THIBAUT SOHIER¹, MARCO GIBERTINI¹, NICOLA MARZARI¹, MATTEO CALANDRA², and FRANCESCO MAURI³ — ¹THEOS and MARVEL, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — ²IMPMC, CNRS, Université Pierre et Marie Curie, Paris, France — ³Departimento di Fisica, Università di Roma La Sapienza, Roma, Italy

The ability to perform first-principles calculations of phonons and electron-phonon interactions in gated 2D heterostructures is crucial to the understanding and design of next-generation devices. Yet, standard methods relying on 3D periodic-boundary conditions fail to properly account for the consequences of dimensionality and the field-effect on electron-phonon physics. Here we present an implementation of density-functional perturbation theory using open boundary conditions adequate to the simulation of 2D systems, and with the possibility to add charged planes to emulate the doping of the slab via field-effect. We first illustrate the importance of working in the correct 2D framework with the study of long-wavelength phonons in polar materials, focusing on two mechanisms relevant for the performances of electronic devices: the Fröhlich interaction and the LO-TO splitting. Second, we address the consequences of the field-effect setup by looking at flexural phonons and their coupling to electrons in gated graphene. We observe that unlike isolated graphene, the coupling with flexural phonons in gated graphene is not forbidden by symmetry, but it is strongly suppressed by electronic screening.

15 min. break.

DS 2.8 Mon 11:30 H 2032

Spectroscopic characterization of the silicene multi-layer phase on Ag(111) — ●DMYTRO SOLONENKO¹, SANDHYA CHANDOLA², EUGEN SPEISER², NORBERT ESSER², DIETRICH R.T. ZAHN¹, and PATRICK VOGT¹ — ¹Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — ²Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., 12489 Berlin, Germany

The formation of so-called “multi-layer silicene” has been suggested to form for supramonolayer Si coverages on Ag(111)[1], but its nature is still controversially discussed including silicene multi-layers, bilayers or Ag-mediated growth of bulk Si with a Ag-terminated ($\sqrt{3} \times \sqrt{3}$)R30° reconstruction[2]. However, the experimental results which were shown so far do not allow an unequivocal assignment of this phase to any of the suggested structures. In order to retrieve the structural properties of this ($\sqrt{3} \times \sqrt{3}$)R30° structure, we carried out an *in situ* Raman spectroscopy study varying the Si coverage (up to 10 monolayers). Our results show a unique spectral signature, which does not bear any resemblance to monolayer epitaxial silicene[3]. We compare the Raman results to those for the ($\sqrt{3} \times \sqrt{3}$)R30° Ag/Si(111) system, yielding the similarities in terms of the overall number of spectral bands and their positions but also suggests fundamental differences, hinting towards the formation of a Si bilayer.

[1] Vogt, P., *et al.*, *Appl. Phys. Lett.* **104**, 021602 (2014). [2] Borenstein, Y., *et al.*, *Phys. Rev. B* **92**, 155407 (2015). [3] Solonenko, D., *et al.*, *2D Mat.* **4**, 015008 (2017).

DS 2.9 Mon 11:45 H 2032

Frictional anisotropy of MoS₂ studied with molecular dynamics simulations — ●VICTOR CLAERBOUT¹, TOMAS POLCAR^{1,2}, and PAOLO NICOLINI¹ — ¹Czech Technical University in Prague, Prague, Czech Republic — ²nCATS, University of Southampton, Southampton, United Kingdom

Transition metal dichalcogenides are considered to be among the best solid lubricants due to their lamellar structure. Tribological research focused upon molybdenum disulfide has revealed its super low friction behavior [1]. However, a full understanding of the mechanism behind this behavior remains lacking. In this contribution we aim to elucidate the phenomena taking place at the nanoscale when two commensurate layers of molybdenum disulfide slide one atop of another. In particular, by means of molecular dynamics simulations, we studied the effect of sliding anisotropy [2] (i.e., the changing frictional behavior upon varying the sliding angle of two commensurate layers) on the energy dissipation due to friction. We simulated different sliding conditions (varying e.g. normal load, sliding speed and system temperature) in order to highlight their effect on the lubricating properties. These results will help on the one hand to identify the fundamental mechanisms that govern friction at an atomistic level, as well as providing

guidelines for the design of novel layered materials with improved tribological properties.

[1] J.M. Martin *et al.*, *Phys. Rev. B*, **48**, 10583(R) (1993). [2] Onodera *et al.*, *J. Phys. Chem. B*, **114**, 15832 (2010).

DS 2.10 Mon 12:00 H 2032

Structural changes and phase stability of Ti doped MoS₂ monolayers — ●ANDREA SILVA, TOMAS POLCAR, ONDREJ HOVORKA, and DENIS KRAMER — Faculty of Engineering and Environment, University of Southampton, SO17 1BJ Southampton, United Kingdom

The discovery of graphene and its remarkable properties has renewed interest in inorganic materials and drawn attention to two-dimensional systems. Transition metal dichalcogenides (TMDs) have been known for decades in industry, but only recently their graphite-like layered structure has renewed academic interest. Quantum confinement in the monolayers yields different electronic properties compared to bulk counterparts. Moreover, TMDs are more chemically versatile than graphene, allowing easy functionalization of the layers [1]. Understanding the doping possibilities for TMDs is a key step in exploiting their potential.

In this study, we focus on the Ti doped MoS₂ TMD, a recently proposed new material with enhanced tribological properties [2].

In order to address the challenging task of determining the phase-stability of a new compound, we map energy landscapes obtained with DFT onto a cluster-expansion hamiltonian and iteratively search for low energy orderings of the atoms inside the given host. This methodology allows us to explore the Ti-Mo-S phase space and determine doping possibilities leading to stable phases of the form Ti_xMo_{1-x}S₂, quantify miscibility gaps and thermodynamic competition with ternary oxides.

[1] M. Chhowalla *et al.*, *Nat. Chem.* **5**, 263 (2013).

[2] A. Cammarata and T. Polcar, *Inorg. Chem.* **54**, 5739 (2015).

DS 2.11 Mon 12:15 H 2032

Resonance profiles of valley polarization in single-layer MoS₂ and MoSe₂ — ●HANS TORNAZKY¹, ROLAND GILLEN^{1,2}, ANNE-MARIE KAULITZ¹, and JANINA MAULTZSCH^{1,2} — ¹Institut für Festkörperphysik, TU Berlin, Germany — ²Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Transition metal dichalcogenides (TMDCs) attract a lot of interest due to their unique properties, such as the repeatedly investigated strong photoluminescence from the direct gap in few layered samples. Furthermore, TMDCs have recently become promising materials for spin- and valleytronics as circular polarized excitation leads to the generation of electron-hole-pairs with distinct spin at either *K* or *K*^{*} points in the Brillouin zone. However, questions remain unanswered about the mechanisms of the scattering processes.

In this talk we present photoluminescence measurements with different excitation energies on single-layer MoS₂ and MoSe₂ in order to examine the resonance behavior of the conservation of circular polarization in these TMDCs. We find that the circular polarization of the emitted light is conserved to 100% in MoS₂ and 84%/79% (*A/A*⁻ peaks) in MoSe₂ close to resonance. The values for MoSe₂ surpass any previously reported value. However, in contrast to previous predictions, the degree of circular polarization decreases clearly at energies less than the 2 LA phonon energy above the resonance.

Our findings indicate that at least two competing processes underly the depolarization of the emission in single-layer transition metal dichalcogenides.

DS 2.12 Mon 12:30 H 2032

Defect mediated phase transformation of two-dimensional 2H-MoTe₂ to the distorted 1T'-MoTe₂ — ●TIBOR LEHNERT¹, MAHDI GHORBANI-ASL², JANIS KÖSTER¹, HANNU-PEKKA KOMSA³, ARKADY KRASHENINNIKOV^{2,3}, and UTE KAISER¹ — ¹Electron Microscopy Group of Materials Science, University of Ulm, Ulm 89081, Germany — ²Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden 01328, Germany — ³Department of Applied Physics, Aalto University, P.O. Box 11100, 00076 Aalto, Finland

We applied the newly developed Cc- and Cs-corrected SALVE (Sub-Angstrom Low-Voltage Electron Microscopy)[1] instrument, to study the dynamics of extended defects in single-layer 2H-MoTe₂. In particular we report atom by atom on the transformation of an area in single-layer MoTe₂ from the semiconducting 2H to the distorted and metallic 1T'^{*} phase, starting with a single vacancy line of missing Te atoms. We find that the size of the transformed area is defined by

the length of the single vacancy line. First-principles calculations are performed to understand the transformation's driving forces.

[1] www.salve-project.de

DS 2.13 Mon 12:45 H 2032

Excitonic transitions in heterostructured Mo and W transition metal dichalcogenides from first principles — ●ROLAND GILLEN and JANINA MAULTZSCH — Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Novel two-dimensional materials from the group of layered transition metal dichalcogenides (TMDC) attract scientific interest for their unusual physical properties, such as their strong optical response. Two ways to tailor the electronic and optical properties are (i) the combination of different TMDCs to form lateral and stacked heterostructures and (ii) creation of alloys containing different metal or chalcogen atoms. Recent experiments have suggested long-lived interlayer excitons in stacked heterostructures, with spatial separation of electrons and holes across the layers, allowing for exploitation in solar cells.

Based on recent work [1,2], we show the theoretical absorption spectra of bilayer MoSe₂-WSe₂ and MoS₂-WSe₂ heterostructures from solution of the excitonic Bethe-Salpeter equation with GW quasiparticle corrections and inclusion of spin-orbit-coupling. In accordance with experimental observations, we find contributions related to interlayer excitons below the absorption onset of the monolayer materials. Our calculations allow us to estimate the binding energy of these electron-hole pairs to be on the order of 0.2 eV for both studied heterostructures. We will further show recent calculations of the absorption spectra of alloyed MoWS₂ materials.

[1] Gillen et al., IEEE JSTQE 23, 1 (2017), [2] Gillen et al., in

preparation

DS 2.14 Mon 13:00 H 2032

Suppression of inhomogeneous broadening of excitons and trions in encapsulated MoSe₂ monolayers — ●MAX WALDHERR¹, JACOB GODDARD¹, NILS LUNDT¹, SEFAATTIN TONGAY², KENJI WATANABE³, TAKASHI TANIGUCHI³, SVEN HÖFLING^{1,4}, and CHRISTIAN SCHNEIDER¹ — ¹Technische Physik, Physikalisches Institut and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — ²School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, Arizona 85287, USA — ³National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — ⁴SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Two-dimensional transition metal dichalcogenides offer a rich platform for the investigation of light-matter coupling effects due to unique effects such as spin-valley locking. In the monolayer limit the optical properties of these materials are highly sensitive to surface effects, hence the exciton and trion resonances undergo inhomogeneous broadening by surface impurities. We present a method to reduce the linewidth of these resonances involving encapsulation between two ultra-thin hexagonal boron nitride layers and thermal annealing in an argon-hydrogen atmosphere. With this technique inhomogeneous broadening is suppressed effectively which manifests in a Lorentzian line shape and improved optical quality. Moreover, the spectral weight of the exciton increases and the linewidths of the exciton and trion reduce to 2.9 and 2.4 meV, respectively.