O 48: 2D Materials 1: Electronic Structure of Transition Metal Dichalcogenides

Time: Wednesday 15:00–17:30 Location: S052

O 48.1 Wed 15:00 S052

the stability of point defects in 2D monolayer transition metal dichalcogenides and their impact on the electronic structure — •ALAA AKKOUSH[1,2] and MARIANA ROSSI[1,2] — [1]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, Berlin — [2]MPI for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22765 Hamburg

Defects can strongly influence the electronic, optical and mechanical properties of 1D materials. However, their stability and distribution under different conditions of temperature, pressure and strain are not well characterized from an atomistic perspective. We have investigated the structural and electronic properties, as well as the thermodynamic stability of point defects (vacancies and adatoms) in monolayer transition metal dichalcogenides MX_2 with M=Mo/W and X= S/Se, through density-functional theory (DFT) simulations with hybrid exchange correlation functional, as implemented in the all-electron package FHI-aims [1]. These calculations are carried out using a supercell approximation to model localised defects using periodic boundary conditions. We show quantitatively that X adatom is most favorable in rich X conditions while in poor X environment X monovacancy is most favorable. Interestingly, an interplay between adatom and divacancies takes place as temperature increases. To gauge the importance of vibrational free energy contributions on the engineering of gap states in the 2D monolayers, we compare the formation energies of point defects with an adsorbed F6TNAP at various thermodynamic conditions.

[1] S.V. Levchenko , et al., *Comp. Phys. Comm.* **192** 60-69 (2015)

O 48.2 Wed 15:15 S052

Non-linear optical response of TMD Nanotubes using Wannier interpolation — •JYOTI KRISHNA and JULEN IBAÑEZ-AZPIROZ — Centro de Fisica de Materiales (CSIC-UPV/EHU), Donostia-San Sebastian, Spain

Single crystals lacking an inversion center display a non-vanishing second-order response known as shift current- a dominant contribution to the bulk photovoltaic effect. There has been a renewed interest in novel materials with large non-linear absorption capabilities[1]. Here we focus on transition metal dichalcogenide nanotubes, which have recently exhibited a short-circuit intensity showing orders of magnitude enhancement over the monolayer value[2]. We systematically explore the implications of the different chiral indexes on both linear and quadratic optical responses for single-walled TMD NT employing the Wannier interpolation technique. We classify the allowed symmetry and calculate the dependence of the magnitude of the response as a function of NT diameter and chirality. Finally, we discussed our results in the context of the experimental measurements.

Funding provided by the European Union's Horizon 2020 research and innovation programme under the European Research Council (ERC) grant agreement No 946629. (1) L. Z Tan, F. Zheng, F. Wang and A. M. Rappe, npj Comput. Mater. 2, 16026 (2016). (2) Y. J. Zhang et. Al Nature 570, 349 (2019). (3) G. Pizzi et. Al, J. Phys. Cond. Matt 32, 165902 (2020).

O 48.3 Wed 15:30 S052

Structural, electronic and optical properties of strained MoS_2 — •JAN-HAUKE GRAALMANN and MICHAEL ROHLFING — Institute of Solid State Theory, University of Münster, 48149 Münster, Germany

Experimental and theoretical studies have shown that the spectrum of MoS_2 changes when the system gets strained. Stretching a monolayer leads to a shift of the optical absorption spectrum to lower energies. In case of the bilayer under hydrostatic stress, the interlayer interaction plays a major role.

In this talk we investigate the behaviour of a MoS_2 monolayer and bilayer theoretically using DFT, *GdW* and the Bethe-Salpeter equation. Our results show a transition of the monolayer from a direct semiconductor to an indirect one when the in-plane lattice constant is increased. Furthermore, the fundamental gap at the K point is reduced while the binding energies of the A and B excitons remain approximately constant. These effects lead to an effective shift of the excitation energies of both excitons towards lower energy with similar gauge factors.

We also find a significant influence of interlayer interaction within the bilayer. The effect of a decreasing gap by biaxial shrinking of each single layer under an external hydrostatic pressure gets counterbalanced by the reduction of the interlayer distance.

O 48.4 Wed 15:45 S052

Excitons in TMDC Bilayers — •JAN NELLESEN and MICHAEL ROHLFING — Westfälische Wilhelms-Universität, Münster, Germany

Semiconducting Transition-Metal-Dichalcogenides (TMDCs) have gained a lot of attention in the past few years due to possible new applications in optoelectronics. In particular, the excitonic properties of TMDC mono- and bilayers have been studied extensively.
This work focuses on interlayer excitons in TMDC heterostructures which combine large binding energies with relatively long lifespans. The exciton energies are investigated in different systems using the Bethe-Salpeter-Equation.
In order to describe excitons in twisted bilayers, which exhibit long-range moiré structures, *ab initio* approaches are no longer feasible because of their high computational demand. With the goal of studying excitons in such systems in mind, the TMDC bandstructure is modeled within a tight-binding approximation. For describing the electron-hole interaction, a model potential is used.

O 48.5 Wed 16:00 S052

Unoccupied electronic states of 1T-$TiSe_2$: Band dispersions and CDW-induced changes at $\overline{\Gamma}$ — •PATRICK GEERS, MARCEL HOLTMANN, and MARKUS DONATH — University of Münster, Germany

The transition metal dichalcogenide 1T-$TiSe_2$ shows a phase transition into a charge density wave (CDW) below a critical temperature T_{CDW} [1]. This transition leads to a half-sized Brillouin zone and backfolded electronic bands. For the occupied electronic structure, photoemission results show a backfolding of Se-$4p_{x,y}$ valence bands below T_{CDW} from $\overline{\Gamma}$ to $\overline{M}$ [2].
We present angle-resolved inverse-photoemission (IPE) measurements for the unoccupied electronic structure above and below T_{CDW}. Our data for the $\overline{\Gamma}\,\overline{M}$ azimuth resemble literature data for the energy vs. momentum dispersion of Ti-3d states as well as an image-potential-induced surface state [3]. In addition, we report on IPE measurements for the $\overline{\Gamma}\,\overline{K}$ azimuth. Finally, we give special attention to the changes in the electronic structure, which are caused by the CDW phase transition. Measurements around $\overline{\Gamma}$ below T_{CDW} show modifications in the spectra which are attributed to backfolded electronic bands from $\overline{M}$ to $\overline{\Gamma}$ as a direct consequence of the CDW phase.

[1] Di Salvo *et al.*, Phys. Rev. B **14**, 4321 (1976).
[2] Watson *et al.*, Phys. Rev. Lett. **122**, 076404 (2019).
[3] Drube *et al.*, J. Phys. C **20**, 4201 (1987).

O 48.6 Wed 16:15 S052

Nontrivial Doping Evolution of Electronic Properties in Ising-Superconducting Alloys — •WEN WAN[1], DARSHANA WICKRAMARATNE[2], PAUL DREHER[1], RISHAV HARSH[1], IGOR I. MAZIN[3], and MIGUEL UGEDA[1] — [1]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain — [2]Center for Computational Materials Science, U.S. Naval Research Laboratory, Washington, DC 20375, USA — [3]Department of Physics and Astronomy, George Mason University, Fairfax, VA 22030, USA

TMDs offer unprecedented versatility to engineer 2D materials with tailored properties to explore novel structural and electronic phase transitions. Here, we present the atomic-scale evolution of the electronic ground state of a monolayer of Nb1-δMoδSe2 ($0<\delta<1$) using STM/STS measurements at 300 mK. We investigate the atomic and electronic structure of this 2D alloy throughout the metal to semiconductor transition (NbSe2 to MoSe2). Our measurements let us extract the effective doping of Mo atoms, the bandgap evolution and the band shifts, which are monotonic with δ. Furthermore, we demonstrate that collective phases (CDW and superconductivity) are remarkably robust against disorder. We further show that the superconducting TC changes non-monotonically with doping. This contrasting behavior in the normal and superconducting state is explained using first-principles calculations. We show that Mo doping decreases the DOS at EF and the magnitude of pair-breaking spin fluctuations as a function of Mo content. (1) W. Wan, et al. Advanced Materials, accepted (2022).

O 48.7 Wed 16:30 S052

Surface spin texture derived from a single mirror plane of WTe_2 — Tristan Heider[1], Gustav Bihlmayer[2], Jakub Schusser[3,4], Friedrich Reinert[4], Jan Minar[3], Stefan Blügel[2], Claus M. Schneider[1], and •Lukasz Plucinski[1] — [1]PGI-6 Forschungszentrum Jülich — [2]PGI-1 Forschungszentrum Jülich — [3]University of West Bohemia, Pilsen, Czech Republic — [4]Experimentelle Physik VII, Universität Würzburg

WTe_2 is an important semi-metallic quantum material that exhibits non-saturating magnetoresistance and potentially hosts Weyl type-II nodes [1]. Through the laser-driven spin-polarized ARPES Fermi surface mapping, we demonstrate highly asymmetric spin textures of electrons photoemitted from the surface states of WTe_2. Such asymmetries are not present in the initial state spin textures, which are bound by the time-reversal and crystal lattice mirror plane symmetries. The findings are reproduced qualitatively by theoretical modeling within the one-step model photoemission formalism, while a simple toy-model suggests that a similar effect shall be observed in other materials with low symmetry.

Our spin-polarized maps with detail comparable to the previous spin-integrated maps [2] have been measured using the newly developed high-resolution instrument at PGI-6 in Jülich that is based on a hemispherical analyzer with the scanning lens, an exchange-scattering spin detector, and a *cw* 6 eV laser.

[1] P. K. Das et. al. Electron. Struct. 1, 014003 (2019) and refs. therein. [2] F. Y. Bruno et al., Phys. Rev. B 94, 121112 (2016).

O 48.8 Wed 16:45 S052

Effect of gold substrate on the excitonic properties of MoS_2: a final state sum frequency spectroscopy study — •Tao Yang, Erik Pollmann, Stephan Sleziona, Marika Schleberger, Richard Kramer Campen, and Yujin Tong — Fakultät für Physik Universität Duisburg-Essen, 47057 Duisburg, Germany

Monolayer transition metal dichalcogenides(TMDCs) are promising candidates for applications in electronics, optoelectronics, and photocatalysts due to their good thermodynamic stability, ease of preparation, tunable bandgap in the visible region, and pronounced activity for photoelectrochemical water splitting. To take advantage of their excellent properties to build the devices and catalysts, a metallic surface is required to combine them. However, compared to the well-explored properties of monolayer TMDCs on dielectric substrates, less attention has been paid to these properties on metal substrates due to the challenges associated with linear spectroscopies probing, such as quenching. Here we use a final state sum frequency spectroscopy(FSSFG) to study the optical properties of MoS_2 exfoliated on a gold surface. Relative to the well-known six-fold symmetry of MoS_2 on SiO_2, the azimuthal dependent FSSFG show significantly different patterns at different polarization combinations. The current study provides important insights into the significant changes in electronic structure when MoS_2 comes into contact with gold, and the possibility to selectively switch resonance on and off through azimuthal tuning, as revealed by the robust FSSFG.

O 48.9 Wed 17:00 S052

Time-resolved momentum microscopy of moiré interlayer excitons in twisted TMD heterostructures — •David Schmitt[1], Jan Philipp Bange[1], Wiebke Bennecke[1], AbdulAziz AlMutairi[2], Giuseppe Meneghini[3], Daniel Steil[1], R. Thomas Weitz[1], Sabine Steil[1], G. S. Matthijs Jansen[1], Samuel Brem[3], Ermin Malic[3], Stephan Hofmann[2], Marcel Reutzel[1], and Stefan Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, Göttingen, Germany — [2]Department of Engineering, University of Cambridge, Cambridge CB3 0FA, U.K. — [3]Fachbereich Physik, Philipps-Universität, 35032 Marburg, Germany

Transition metal dichalcogenides (TMDs) are extensively studied because of their exceptional material properties. The stacking of different TMDs can lead to even more intriguing electronic properties: In type-II band aligned TMD stacks, novel excitonic states can be created where the electron and the hole contribution to the exciton are separated between the van-der-Waals-coupled TMDs. A twist angle between these layers allows further manipulation of the electronic properties and gives rise to moiré-patterns which leads to distinct patterns in momentum space. Here, we make use of our setup for time-resolved momentum microscopy that is perfectly suited to probe these excitonic features with energy- and in-plane momentum resolution. We present femtosecond evaluation of the momentum-fingerprints of the excitonic features that are created on a type II aligned heterostructure. Schmitt *et al.*, arXiv:2112.05011 (2021).

O 48.10 Wed 17:15 S052

***In Operando* Soft X-Ray Photoemission Spectroscopy of 2D Material Devices** — •Alena Nierhauve[1,2], Matthias Kalläne[1,2], Tammo Zimmermann[1], Jens Buck[1,2], Philipp Kagerer[3], Zhansong Geng[4], Chao Zhang[4], Frank Schwierz[4], Martin Ziegler[4], Rok Venturini[5], and Kai Rossnagel[1,2,6] — [1]IEAP, CAU Kiel, 24098 Kiel, Germany — [2]Ruprecht-Haensel-Labor, DESY and CAU Kiel, 22607 Hamburg and 24098 Kiel, Germany — [3]Dep. of Exp. Physics VII, JMU Würzburg, 97074 Würzburg, Germany — [4]Dep. of Electr. Engineering and Information Techn., TU Ilmenau, 98684 Ilmenau, Germany — [5]Jožef Stefan Institute, 1000 Ljubljana, Slovenia — [6]DESY, 22607 Hamburg, Germany

Layered transition-metal dichalcogenides (TMDCs) are a particularly promising platform for low-dimensional electronic devices due to their two-dimensional nature and richness regarding physical phenomena. This includes non-linear conductance behavior due to, e.g., metal-insulator transitions and memristive behavior, which is of particular interest to in-memory computing designs for neuromorphic systems. By combination of micrometer position- and angle-resolved photoemission spectroscopy (μ-ARPES) in the soft X-ray range with *in operando* electrical control, we attempt to study the electronic structure changes concomitant with thickness changes and non-equilibrium conditions in device-like structures based on TMDCs. A portrayal of conductance-governing mechanisms at a fundamental level could help to evolve towards the understanding and engineering of novel band structures, transport phenomena, and device functionality.