Anisotropy in optical properties of GeS and GeSe

<u>Agata Tołłoczko,</u> Szymon J. Zelewski, Michał Błaszczak, Tomasz Woźniak, Paweł Scharoch, Robert Kudrawiec

Department of Semiconductor Materials Engineering, Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

Group-IV monochalcogenides (MXs), such as GeS, GeSe, SnS, and SnSe, are semiconducting van der Waals crystals isoelectronic to black phosphorus, with superior stability in air conditions [1]. They crystalize in the orthorhombic structure, with characteristic puckered atomic arrangement along one of the crystallographic directions, which results in strong in-plane anisotropy [2,3]. High optical absorption, good conductivity, and band gaps ranging from 1 to 2 eV make these materials suitable for applications in photovoltaics and light detection [3,4,5], however their optoelectronic properties are not yet fully understood.

In our research we investigate fundamental properties of MXs by means of optical spectroscopy, supported by theoretical DFT calculations of the electronic band structure. Our experimental results obtained for GeS and GeSe show that the optical properties of these materials are dominated by direct transitions. The fundamental band gap, however, might be in fact indirect, and was not observed in the experiments due to closely lying direct transitions, as they are characterized by higher oscillator strength. Such interpretation coincides with our calculations, providing the picture of the Brillouin zone with multiple band extrema in close energy proximity, as reported in our recent work [7]. In order to investigate the anisotropy of GeS and GeSe, polarization-resolved measurements have been performed, revealing strong dependence of the observed optical transitions on the light polarization.

- [1] L. C. Gomes, A. Carvalho, Phys. Rev. B, 92, 085406 (2015)
- [2] D. Tan et al., Nano Res., 10(2), 546–555 (2017)
- [3] L. Huang et al., J. Chem. Phys. 144, 114708 (2016)
- [4] R. Ulaganathan et al., Nanoscale, 8, 2284-2292 (2016)
- [5] P. Zhao et al., J. Mater. Chem. A, 5, 24145-24152 (2017)
- [6] P. A. E. Murgatroyd et al., Chem. Mater., 32, 3245–3253 (2020)
- [7] A. Tołłoczko *et al.*, Mater. Adv., **1**, 1886-1894 (2020)