Metal Chalcogenides for Thermoelectricity, Solar Cells and Optoelectronic Devices

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Searching the new materials with desired properties and optimization of their synthesis methods is one of very important directions of physics development. It allows to get research objects to verify new hypotheses or confirm predictions of advanced theoretical concepts (e.g. topological materials $Pb_{1-x}Sn_xSe$). From the other hand, concerning the engineering materials, it is important to obtain optimal, desired properties (efficiency, durability, non-toxicity, manufacturing costs) for particular applications.

In my talk I focus on establishing the fundamental relationship between chemical composition, crystallographic structure and physical properties (thermoelectricity, NLO, solar cells, dosimetry, Mid-Red luminescence) and then I would like to explain laser stimulated effects such as change in absorption, piezo-optical properties, intensity of the second and third harmonics of light or the phenomenon of luminescence. This allowed to determine which chemical bonds or kind of defects and their concentration in the crystallographic structure have a crucial influence on the observed relationships. This knowledge gives the possibility of introducing effective modifications of particular compounds by creating new crystals, solid solutions, doping, low dimensionality and improving the growth technology in order to achieve the desired properties.

An important element of the lecture will be the issue of chalcogenide single crystals for which we additionally conducted comprehensive studies of crystallographic and electronic structures using the XRD method, XPS and XES photoelectron spectroscopy. Because the XPS and XES studies allow to determine not only the total density of electron states in the valence band, but also the partial contribution to total density of states from individual atoms, after DFT calculations it is possible to check the agreement between the calculated and experimental data. In addition, I put a special emphasis on the experimental determination of the band gap, activation energy and their dependence on temperature, structure of defect etc., which is also an additional important procedure to verify the prediction of computational methods. I will discuss and compare between the results of calculations with relevant optical measurements performed in a wide spectral range, NLO effects, photoconductivity and piezo-optics. In convincing manner, I demonstrate that the electron properties and material constants of chalcogenide crystals can be changed in a wide range by means of laser irradiation (the photo-induction process), tune composition, changes of structure and nano-effects.

Partially supported by National Science Centre (NCN) 2018/31/B/ST4/00924, 2021/40/Q/ST5/00336