Layered $AgInP_2S_6$ semiconductor: insight into properties of the $Me1Me2P_2X_6$ crystalline family

T. Babuka[1,2], K. Glukhov[2], M. Makowska-Janusik[1], Yu. Vysochanskii[2]

[1]Faculty of Mathematics and Natural Science, *Institute of Physics, Jan Dlugosz University in Czestochowa, Al. Armii Krajowej 13/15, 42200 Czestochowa, Poland*
[2]*Institute for Solid State Physics and Chemistry, Uzhgorod National University, 54 Voloshyn St., 88000 Uzhgorod, Ukraine*

Hexachalcogenohypodiphosphates have attracted great attention in the past years due to their interesting physical and chemical properties. The layered crystals of the $Me1Me2P_2X_6$ (Me1, Me2 – metal cations, X – chalcogen) family are promising materials for functional electronics [1]. In presented work physical properties of the $AgInP_2S_6$ crystal [2] will be discussed because according to our knowledge, information about mentioned pure crystals is almost absent in the literature.

In this case, using first principle calculations the structural, electronic, vibrational and elastic properties of the $AgInP_2S_6$ were studied. Detailed structural and symmetry analysis of $AgInP_2S_6$ crystal were carried out using DFT-D approach. The properly used combination of the DFT methodology and Grimme correction give opportunely to carried out correctly geometry optimization of the considered layered structure. The energy band spectrum of the studied crystal was calculated for the first time. Using GGA-D approximation the values of the band gap of the $AgInP_2S_6$ crystal was calculated to be equal 1.02 eV. To explain the nature of chemical bonding existing in layered chalcogenide crystals DOS, COOP/COHP, Wannier orbitals and spatial distribution of electron density were calculated. As the result was shown that the role of *d*-orbitals located at Ag and In cations is completely different. The *d*-electrons of In atoms form more stable and localized charge distribution, while self-overlapping of Ag orbitals makes them more labile and facilitate their delocalization and exchange (possibly indirect) with neighboring atoms.

Performed investigations help better carried out computer simulations of vibrational properties. The calculated data were compared with the available experimental results on Raman scattering and a satisfactory agreement was demonstrated. Elastic anisotropy (directional dependence of the Young moduli) of these compounds was modeled and analyzed for the first time. Using the Christoffel equation the sound velocity of $AgInP_2S_6$ crystal in the plane of the layers (001) was obtained to be equal to 3204.4 m/s.

Finally, the results of performed investigations confirm that $AgInP_2S_6$ crystal has promising physical properties and can be used for the creation of new functional (artificial) materials.

[1] J. W. Bennett, K. M. Rabe, *Journal of Solid State Chemistry* **195**, 21–31 (2012).
[2] Z. Ouili, A. Leblanc, P. Colombet, *Journal of Solid State Chemistry* **66**, 1, 86-94 (1987).