Effect of pressure of the electronic and optical properties of $In_{4/3}P_2S_6$ crystal: first principle calculations

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Two-dimensional materials are promising candidates for use inphotovoltaic solar cells and for functional electronics. Among the wide variety of 2D materials, layered metal phosphorus trichalcogenides composed of metal cations located between two layers of thiophosphate $(P_2S_6)^{4-}$ atoms through strong ionic bonds have attracted much attention [1, 2]. These ferroelectrics, in principle, can overcome the fundamental scaling problem imposed by the thickness limit, owing to their inherent features of dangling bonds-free surfaces and weak van der Waals (vdW) interlayer couplings [3]. Two-dimensional nanomaterials are well-suitable for strain engineering because they can withstand large strain, and the strain in two-dimensional materials can modify the atomic and electronic structure, optical property.

Previously, the effect of stress on such crystals as $AgInP_2S_6$ [4] and $CuInP_2S_6$ [5] was widely studied. We consider in our research a material close to the above-mentioned crystals. One of the important materials included in this group of crystals is $In_{4/3}P_2S_6$ crystal. Studies of the deformation properties of this material have not been carried out before. Thus, we performed first-principle calculations of the electronic and optical properties of this material at different pressures.

The structural properties such as equilibrium lattice parameters, bulk modulus and its first pressure derivative were obtained using an optimization method. As a result, an equation of state of the Birch-Murnaghan type was obtained. The optical properties of this material, such as dielectric function, refractive index and the optical band gap were also calculated. In addition, the influence of the hydrostatic pressure on the energy band structures and the refractive index of these compounds were investigated. We have calculated the pressure-induced energy shifts and the coefficients of the power-law decomposition of the pressure dependence of the band gap were obtained.

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