

Electronic and Optical Properties of Li₂S Antifluorite Material

Authors : Brahim Bahloul, Khatir Babesse, Azzedine Dkhira, Yacine Bahloul, Dalila Hammoutene

Abstract : In this paper, we investigate with ab initio calculations some structural and optoelectronic properties of Li₂S compound. The structural and electronic properties of the Li₂S antifluorite structure have been studied by first-principles calculations within the density functional theory (DFT), whereas the optical properties have been obtained using empirical relationships such as the modified Moss relation. Our calculated lattice parameters are in good agreement with the experimental data and other theoretical calculations. The electronic band structures and density of states were obtained. The anti-fluorite Li₂S present an indirect band gap of 3.388 eV at equilibrium. The top of the valence bands reflects the p electronic character for both structures. The calculated energy gaps and optical constants are in good agreement with experimental measurements.

Keywords : Ab initio calculations, antifluorite, electronic properties, optical properties

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