World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:12, No:04, 2018

Electronic and Optical Properties of Li_2S Antifluorite Material

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Abstract : In this paper, we investigate with ab initio calculations some structural and optoelectronic properties of Li_2S compound. The structural and electronic properties of the Li_2S 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 Li_2S 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
Conference Title : ICACCM 2018 : International Conference on Advanced Ceramics and Composite Materials
Conference Location : London, United Kingdom
Conference Dates : April 24-25, 2018