Ab Initio Studies of Li_3AlH_6 Materials for Hydrogen Storage Purposes and Optoelectronic Applications

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Hydrogen storage is a definitive step for commercialization of energy production. The solid stated method of hydrogen storge gained much attention in current research, instead of large number of storage thehniques. This research rationally shows the optoelectronic properties of Li_3AlH_6 using computational method. The structrual, density of states and corresponding optical and electrical properties of Li_3AlH_6 was investigated. Firstly, we optimize the crystal structures of solid state Li_3AlH_6 hydrides. Furthermore, electronic and optical band structures of hydrides is computed. The Li_3AlH_6 have indirect bands gap as 2.97 eV (N- Γ). Thus, the investigating material is electronically semiconducting. This indicates that Li_3AlH_6 has a deep influence on its electronic structure and optical properties, which is the goal of theoretical basis for research to be achieved.

Keywords: Hydrogen storage material, Optoelectronic properties, FP-LAPW, DFT.

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