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Electronic structure, optical and thermoelectric transport properties of layered polyanionic hydrosulfate $LiFeSO_4OH$: Electrode for Li-ion batteries

Abstract

Theoretical analysis of electronic structure and optical properties of $LiFeSO_4OH$, using the full-potential linearized augmented plane waves (FPLAPW), on the basis of density-functional theory (DFT), with in the local density approach (LDA), generalized gradient approach (GGA) and Engel–Vosko GGA (EVGGA). Electronic structure and bonding nature of the atoms are investigated in the entire calculation of partial, total density of states and electronic charge densities. The band structure calculations show that the investigated compound is direct band gap semiconductor of about 0.334 eV, 0.580 eV and 1.114 eV. The optical spectra are calculated using EVGGA in the photon energy range up to 13.8 eV. The anisotropic behavior of the imaginary and real parts of the complex dielectric function, reflectivity, refractive index, extension co-efficient and energy loss function are studied for parallel and perpendicular component of electric field polarization. Thermoelectric properties namely, electrical and thermal conductivity, Seebeck co-efficient and power factor are calculated and discussed with the constant relaxation time, using the BoltzTraP code.

Keywords; Electronic structure, Optical properties, Thermoelectric properties, Boltztrap code, EVGGA