Structural, Elastic, Electronic, Magnetic and Thermoelectric Characteristics of $MgEu_2X_4$ (X= S, Se) Spinels

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Abstract

The structural, elastic, electronic, magnetic and thermoelectric properties of $MgEu_2X_4$ (X= S and Se) spinel compounds were investigated computationally. Calculations were performed using the full-potential linearized augmented plane wave (FP-LAPW) method within the Perdew, Burke, and Ernzerhof generalized gradient approximation (PBE-GGA), GGA+U, and modified Becke-Johnson (mBJ-GGA) approximations. The band structure and DOS results from the three exchange-correlation approximation methods (mBJ, GGA+U, and PBE) showed that these spinel compounds were fully spin-polarized. Also, they possess a half-metallic character in the spin-down channel with a direct bandgap (Γ-Γ) of about 3.44 eV, 2.712 eV, and 2.472 eV for $MgEu_2S_4$ and 2.89 eV, 2.285 eV and 2.017 eV for $MgEu_2Se_4$, respectively. The formation of both compounds is energetically favorable based on the results of the total energy and cohesive energy calculations. Furthermore, the two compounds were chemically and mechanically stable, as concluded from cohesive energy and elastic calculations. The elastic calculations revealed that both spinel compounds were ductile materials. The ionic bonds were predominant. The quasi-harmonic model has also been used to investigate the influences of temperature and pressure on some thermal characteristics such as the heat capacity at constant volume, thermal expansion, and lattice thermal conductivity. The thermoelectric behavior was studied using the BoltzTraP code. Both systems showed good thermoelectric properties for the spin-down channel. The main three thermoelectric characters, thermopower (S), power factor (PF), and figure of merit (ZT) at the spin-down channel, were neglected at room temperature (300 K). Their values increased dramatically with increasing the temperature to reach reasonable values at 800 K. These results indicate that both spinels are promising spintronics and thermoelectric applications candidates.