Anomalous thermoelectric properties of new Mn_2ZnSn Heusler compound

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Investigation of thermoelectric properties was carried within the density functional theory by using the classical Boltzmann theory through BoltzTrap code. In the present study, the material shows a direct band gap character in the minority spin channel with a band gap of 0.48 eV. The material presents a ferromagnetic nature with magnetic moment of $2.0 \mu_B$ per formula unit in consistent with Slater Pauling rule. Further we study the thermoelectric properties between the temperature range of 50 K to 800 K. Seebeck coefficient (S) measurements indicate the material as n-type with increasing S value from $13.76 \mu\text{V/K}$ at 800 K to higher temperatures (Figure 1). The material shows higher efficiency with figure of merit equal to 0.99 at 800 K, relatively higher in comparison with the other full Heusler compounds in these temperature ranges (Figure 2). Anomalous thermoelastic properties may lead the material for the use in advanced thermoelectric technology.

Figure 1: Calculated transport coefficient $S \mu\text{V/K}$ as a function of temperature.

Figure 2: Calculated transport coefficient figure of merit zT as a function of temperature

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