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Investigation on Structural, Electronic, Thermal, and Thermoelectric Properties of Co_2MnGa under Pressure Based on Density Functional Theory

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Structural, electronic, thermal, and thermoelectric properties of Co_2MnGa under 0, 5, 10, and 15 GPa pressures have been investigated. In electronic properties, in minority spin, a pseudo band gap (about 0.25 eV) is visible. Thermal properties in the range of 0 to 700 K have been calculated. Our results in thermal properties have a good agreement with another theoretical work. Calculations of thermoelectric properties, in both spin up and down, in the range of 100 to 700 K have been done. In spin up, an abnormal behavior is observed under 5 GPa for electrical conductivity. This is due to increase in Mt at this pressure. The sign and value of Seebeck coefficient in spin up at 300 K has a good consistency with experimental work. Other thermoelectric properties such as: power factor, electronic thermal conductivity divided by relaxation time, electronic contribution of heat capacity at constant volume under pressure have been studied.

Keywords: Co_2MnGa, density functional theory, electronic properties under pressure, thermoelectric properties under pressure.