PAPER ID:163

A PROMISING THERMOELECTRIC RESPONSE OF DIRAC SEMIMETAL Ca_3SnO: A FIRST PRINCIPLE STUDY

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ABSTRACT

The inherent exotic electronic properties of Dirac Semimetals have drawn incredible research consideration in the field of condensed matter physics. The structural and transport properties of Dirac Semimetal Ca_3SnO have been computed by utilising Density Functional Theory (DFT) in combination with Boltzmann transport theory. For the relaxed structure of Ca_3SnO at zero GPa, the values of structural parameters have been calculated. The Seeback coefficient, electrical conductivity, electronic thermal conductivity and thermoelectric power factor have been analysed as a function of chemical potential at 300 K, 600 K, 800 K, 1000 K and 1200 K. The present investigation proposes Ca_3SnO as potential thermoelectric material over the wide range of temperature. The current DFT based calculations would further create a scope of experimental work to explore their technological applications.

Keywords: Dirac Semimetals. Thermoelectric Properties. First principle study. Antiperovskite structure

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