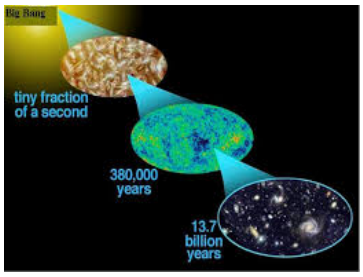

Contribution ID : **16** Type : **not specified**

Study of Spin Polarization, Fermi Surface, Band Structure and Thermophysical Properties of Sc 2 ZrSi Inverse Heusler

вторник, 12 января 2021 г. 16:15 (30)

Study of Spin Polarization, Fermi Surface, Band Structure and
Thermophysical Properties of Sc 2 ZrSi Inverse Heusler
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Abstract
The origin of half-metallicity, spin behavior, thermoelectrics and thermodynamics of inverse full-Heusler Sc 2 ZrSi alloy are explored using the by density functional theory. The structural characterization using the calculation of ground state energy confirm the XA-type structure of Heusler having similarity with Hg 2 CuTi-type structure that has F-43m space group symmetries.Band structure and occupation of density of states at the Fermi level determine its semiconducting nature and an indirect band gap of 0.52 eV.Semi-classical Boltzmann transport theory is used to determine various thermoelectric coefficients to infer about its capability for waste heat recovery systems.The Seebeck coefficient and electrical conductivity measurements also convey semiconducting band structure over all chemical potentials.The thermoelectric efficiency measured through zT calculation with a value of 0.5 at 1200 K, convey the material can be used as thermoelectric material.The thermodynamics using Debye temperature, specific heat and thermal expansion coefficient define low anharmonicity and low lattice thermal conductivity of the material. The overall thermophysical assets suggest the material has a potential stand for spintronics and thermoelectric applications.

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