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Electronic, mechanical and thermoelectric properties of Gd-filled ternary skutterudites

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Rare earth filled ternary skutterudite compounds have potential applications to produce clean energy, long-term stability and low cost as compared to other thermoelectric materials. For good efficiency, materials should possess high electrical conductivity, low thermal conductivity, and high Seebeck coefficient. In this communication, the electronic, mechanical and thermoelectric properties of Gd-filled skutterudites $\text{GdFe}_4\text{P}_{12}$, $\text{GdRu}_4\text{P}_{12}$ and $\text{GdOs}_4\text{P}_{12}$ have been reported. The study is based on full potential linearized augmented plane wave method in the framework of density functional theory. The exchange-correlation potential are treated using the generalized gradient approximation. The electronic behavior of this material is semi-metallic. Investigation of mechanical properties shows that reported materials are brittle and anisotropic. $\text{GdOs}_4\text{P}_{12}$ is stiffest among $\text{GdT}_4\text{P}_{12}$ (T=Fe, Ru, Os). The Boltzmann transport theory with constant relaxation time has been used, as implemented in BoltzTraP code, to predict the thermoelectric properties of all the materials. The magnitude of Seebeck coefficient in spin down channel is more than that in spin up the channel. The maximum values of the figure of merit obtained in spin up channel are 0.44, 0.89 and 0.86 whereas in spin down channel the figure of merit are found to be 0.98, 0.90 and 0.96, respectively for $\text{GdFe}_4\text{P}_{12}$, $\text{GdRu}_4\text{P}_{12}$, and $\text{GdOs}_4\text{P}_{12}$. On the basis of the values of ZT, $\text{GdRu}_4\text{P}_{12}$ is efficient material in spin up configuration and $\text{GdFe}_4\text{P}_{12}$ in spin down configuration. Study of the electronic charge density shows that in the rare earth filled ternary skutterudite compounds have P-P covalent and Gd-B and Fe-B ionic bonding.

Biography

U P Verma has completed His PhD at the age of 25 from Meerut University, Meerut. He is the recipient of Alexander von Humboldt Fellowship at Justus Liebig University, Giessen and Goethe University Frankfurt. He has served as Regional Director of MP Bhoj Open University, Director Institute of Distance Education and as Head, School of Studies in Physics of Jiwaji University, Gwalior. He has published more than 100 research papers in journals of repute and supervised to 18 students for their PhD.

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