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A First principle Study of the Power Factor of phosphorus nitride – a binary Skutterudite

Waste heat generated in most domestic and industrial appliances can lead to fracture or undesirable plastic deformation of materials. Developing new thermoelectric materials or improving the existing ones could be handy in minimizing waste heat. Skutterudites exhibit good electrical and modifiable thermal conductivities making them to be suitable candidates for thermoelectricity. Studies have hinted that skutterudite phosphorus nitride is potentially a thermolelectric material but details remain scanty to date. For more than half a century, emphasis has been placed on the figure of merit (ZT) to pinpoint good thermoelectric. Recently, it has been shown that a material's power factor is more important than the thermal conductivity for thermoelectric power generation for a given ZT. In this work, will calculate the power factor of phosphorus nitride to ascertain its thermoelectric capability. This will be investigated by solving the Boltzmann transport equations using the BoltzTraP code. It is hoped that the outcome of this study may contribute to a better understanding of properties that enhance the efficiencies of thermoelectric materials.

Keywords

Skutterudite, power factor

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