Thermoelectric properties of filled skutterudites from first principles

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It is generally known that the filled skutterudite structure show promising thermoelectric properties in the high temperature regime. This is mainly due to the rattling of the heavy filler atoms at the unfilled positions in the skutterudite structure. We follow recent recommendations and calculate the Seebeck coefficient as a function of temperature for these proposed filled skutterudite structures. The Seebeck coefficient is calculated from Boltzmann theory using the band structure obtained from first principles within the relaxation-time approximation. The validity of this approach is given by a comparison with known experimental values of the Seebeck coefficient.

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