Optical and thermoelectric properties of Tl-filled CoSb₃ skutterudites from first-principles

IN GEE KIM, Northwestern University, ARTHUR J. FREEMAN — Filled skutterudite antimonides have attracted much interest as a new class of thermoelectric materials. We have determined the electronic structures, optical and thermoelectric propertes of Tl-filled skutterudite CoSb₃ by using the highly precise full-potential linearized augmented plane wave (FLAPW) method within the Perdew-Burke-Ernzerhof (PBE) form of the generalized gradient approximation (GGA) to density functional theory. In contrast to the small-gap semiconducting CoSb₃, Tl-filled CoSb₃ is calculated to be metallic with Tl-sp bands strongly hybridized with all the other elements over the entire energy region. The thermoelectric properties, e.g. the Seebeck coefficient, are evaluated and discussed in terms of the diagonal terms of the optical matrix elements.

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