Abstract Submitted
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Optical and thermoelectric properties of Tl-filled $CoSb_3$ skutterudites from first-principles[1] IN GEE KIM, Northwestern University, ARTHUR J. FREEMAN — Filled skutterudite antimonides have attracted much interest as a new class of thermoelectric materials.[2] We have determined the electronic structures, optical and thermoelectric propertes of Tl-filled skutterudite $CoSb_3$ by using the highly precise full-potential linearized augmented plane wave (FLAPW) method[3] within the Perdew-Burke-Ernzerhof (PBE)[4] form of the generalized gradient approximation (GGA) to density functional theory. In contrast to the small-gap semiconducting $CoSb_3$, Tl-filled $CoSb_3$ is calculated to be metallic with Tl-*sp* bands stongly 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.

[1]DARPA Grant B529527
[2]B.C. Sales, D. Mandrus, and R. K. Williams, Science **272**, 1325 (1996).
[3]Wimmer, Weinert, Krakauer, Freeman, Phys. Rev. B **24**, 864 (1981).
[4]Perdew, Burke, Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).

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