Abstract Submitted
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Thermoelectric power generation in ternary skutterudites: a first-principles Wannier-functions' study DMITRI VOLJA, Massachusetts Institute of Technology, MARCO FORNARI, Central Michigan University, BORIS KOZINSKY, Bosch GmbH, NICOLA MARZARI, Massachusetts Institute of Technology — We study from first-principles ternary skutterudites derived from $CoSb_3$, where the pnictogen is substituted with elements from the IVB and VIB groups. We focus on $CoGe_{3/2}S_{3/2}$, $CoGe_{3/2}Te_{3/2}$ and $CoSn_{3/2}Te_{3/2}$, and compute the structure, electronic structure and vibrational properties from density-functional and density-functional perturbation theory. Since the direct evaluation of transport quantities in the relaxation-time approximation is computationally demanding, we use maximally-localized Wannier functions (MLWFs) for accurate integrations of operators across the Brillouin zone. This MLWFs basis leads to a very efficient and well-conditioned scheme to calculate the thermoelectric transport coefficients and to disentangle and identify the contribution of single bands. In addition, it provides a detailed, transferable picture of bonding in these complex materials.

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