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Predicting the Influence of Secondary Phases on the Thermoelectric Performance in Cobalt Containing Spinels (ACo_2O_4; A={Co,Ni,Zn})
TERENCE MUSHO, ANVEEKSH KONERU, DAVID MEBANE, West Virginia University — A promising new compositional space comprised of cobalt containing spinels bound by three end-members, $Co_2(Co)O_4$, $Co_2(Ni)O_4$ and $Co_2(Zn)O_4$, has brought to issue the presence of secondary phases (CoO, NiO, ZnO). These secondary phases are a result of not achieving a complete solid solution across the compositional space. It is hypothesized that under controlled fabrication the geometry and dispersion of these secondary phase can be leveraged to not only limit phonon transport but possibly increase electrical transport resulting in enhanced thermoelectric performance. To understand the influence of these secondary phases, a computational model has been developed that relies on a two dimensional non-equilibrium Green's function (NEGF) formalism to predict both the electrical and thermal contributions to the overall thermoelectric performance. This presentation will discuss the electrical and thermal transport models and approaches taken to incorporate dissipative carrier mechanisms into the quantum models. In addition, computational results predicting the optimal geometry and spacing of the secondary phases will be discussed. In closing, remarks will be made on how these models are currently being integrated into a high-throughput framework for materials discovery.

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