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Investigation of first principle thermoelectric properties of compound semiconductor CEM SEVIK, ALPER KINACI, TAHIR CAGIN, Artie McFerrin Dept of Chemical Engineering, Laboratory of Computational Engineering of Nanomaterials Texas A&M University, College Station, TX, TEXAS A&M UNIVERSITY TEAM — We analyze relevant electronic and transport properties of several different compound semiconductors, Cu_2ZnSnX_4, (X = S, Se, Te), $Cu_2CdSnSe_4$, and Cu_3SbM_3, (M = Se, S) to assess their potential as thermoelectric materials. Using density functional theory and Boltzmann transport equations, we determine Seebeck coefficients, conductivities, and power factors for each compound. To assess their potential application as thermoelectrics, we calculated a simple measure: "maximum" thermoelectric figure of merit, ZT_{max} at experimentally amenable doping levels. We compared this with results for other well known bulk thermoelectrics (Bi_2Te_3 and $SrTiO_3$). However, our calculations indicate that it is not possible to reach ZT values higher than 1, so that these materials to be competitive with other materials for power generation and refrigeration applications.

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