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Alkaline earth lead and tin compounds Ae_2Pb, Ae_2Sn, Ae=Ca,Sr,Ba, as thermoelectric materials DAVID PARKER, DAVID SINGH, Oak Ridge National Laboratory — We present a detailed theoretical study of three alkaline earth compounds Ca_2Pb, Sr_2Pb and Ba_2Pb, which have undergone little previous study, calculating electronic band structures and Boltzmann transport and bulk moduli using density functional theory. We also study the corresponding tin compounds Ca_2Sn, Sr_2Sn and Ba_2Sn. We find that these are all narrow band gap semiconductors with an electronic structure favorable for thermoelectric performance, with substantial thermopowers for the lead compounds at temperature ranges from 300 to 800 K. For the lead compounds, we further find very low calculated bulk moduli - roughly half of the values for the lead chalcogenides, suggestive of soft phonons and hence low lattice thermal conductivity. All these facts indicate that these materials merit experimental investigation as potential high performance thermoelectrics. We find good potential for thermoelectric performance in the environmentally friendly stannide materials, particularly at high temperature.

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