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Carrier Pocket Engineering to Improve Thermoelectric Transport in Semiconducting PbTe

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High Seebeck coefficient in semiconductors generally results from a high density of states (DOS) effective mass. Many unconventional electronic structures that increase DOS are being studied or proposed for high efficiency thermoelectric materials. For example, resonant DOS enhancement demonstrated in Tl doped PbTe increases the Seebeck coefficient and the material has high thermoelectric figure of merit, zT , at high temperature. However high band mass of the carriers results in low mobility, which leads to lower zT . Instead, high DOS effective mass due to high valley degeneracy leads to high zT . For example, utilizing the high degeneracy second valence band in PbTe leads to nearly twice the zT ($zT \sim 1.4$) than that of the first valence band. By engineering the two valence bands to converge further increases the degeneracy and zT .