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Highly effective Mg_9Si_5 thermoelectric for mid temperature applications VIJETA SINGH, JIJI PULIKKOTIL, CSIR- National Physical Laboratory — Commercial acceptance of a thermoelectric device relies not only on its figure of merit (ZT), but also on its cost and environmental friendliness. In this regard, Mg_2Si is a potential candidate system. However, the low solubility of substituents in Mg_2Si severely restricts its optimization and applicability in the energy. Recently a new compound, Mg_9Si_5, had been synthesized. The material accommodates a variety of dopants with varying doping concentration. Using density functional theory based calculations and Boltzmann transport theory we study the electronic structure and transport properties of Mg_9Si_5. We find Mg_9Si_5 is a 0.17 eV semiconductor exhibiting appreciable characteristic properties of a mid-temperature thermoelectric. Based on an empirical estimate, we find its ZT to be approximately 1.1, at an operable temperature of 600 K.

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