

Abstract Submitted  
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**Thermoelectric properties of Mg<sub>2</sub>(Ge, Sn) solid solutions**<sup>1</sup> JIFENG SUN, DAVID J. SINGH, University of Missouri — Intermetallic compounds Mg<sub>2</sub>X (X = Si, Ge, Sn) and their solid solutions have attracted much attention as they are composed of environmental friendly and naturally abundant constituent elements and can be promising thermoelectric materials at intermediate temperature range (500 K - 1000 K). The figure of merit (ZT) of n-type Mg<sub>2</sub>X solid solutions can reach up to 1.5. However, the p-type materials have much lower ZT values up to 0.38. In this talk, we will present the evolution of the thermoelectric properties of Mg<sub>2</sub>(Ge, Sn) solid solutions with a typical composition of Mg<sub>2</sub>Ge<sub>0.5</sub>Sn<sub>0.5</sub> using first principles calculations combining with the experimental data. The ZT was optimized with respect to both doping concentrations and operating temperatures. Importantly, at 500 K - 1000 K temperature range we find ZT values up to 2 are possible for optimized n-type material within 10<sup>19</sup> cm<sup>-3</sup> to 10<sup>20</sup> cm<sup>-3</sup> carrier concentrations. But the p-type counterparts show inferior performance with ZT values ranging from 0.2 to 0.7.

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