Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting information

Efficient Lanthanide Gd Doping Promoting Thermoelectric Performance of Mg_3Sb_2-based Materials

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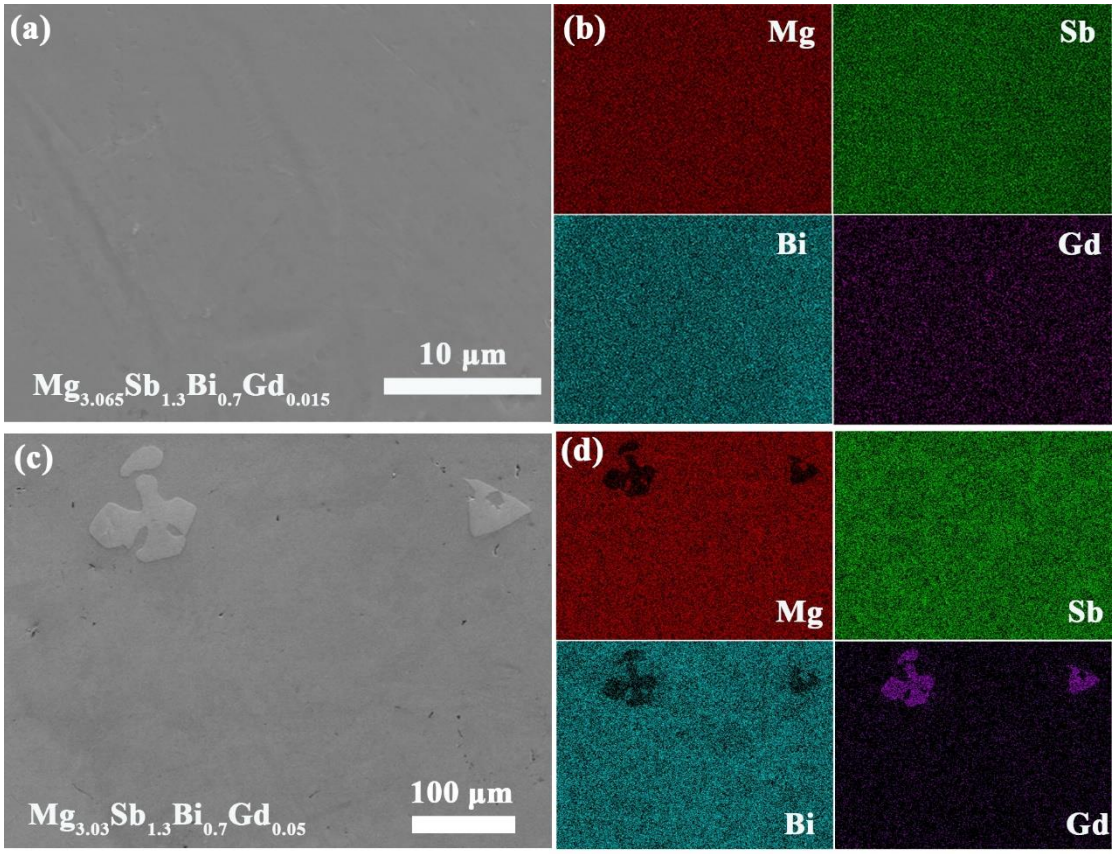

Fig. S1 Backscattering scanning electron microscopy (BSE) images and (b) corresponding EDS mapping for $Mg_{3.065}Sb_{1.3}Bi_{0.7}Gd_{0.015}$ and $Mg_{3.03}Sb_{1.3}Bi_{0.7}Gd_{0.05}$.

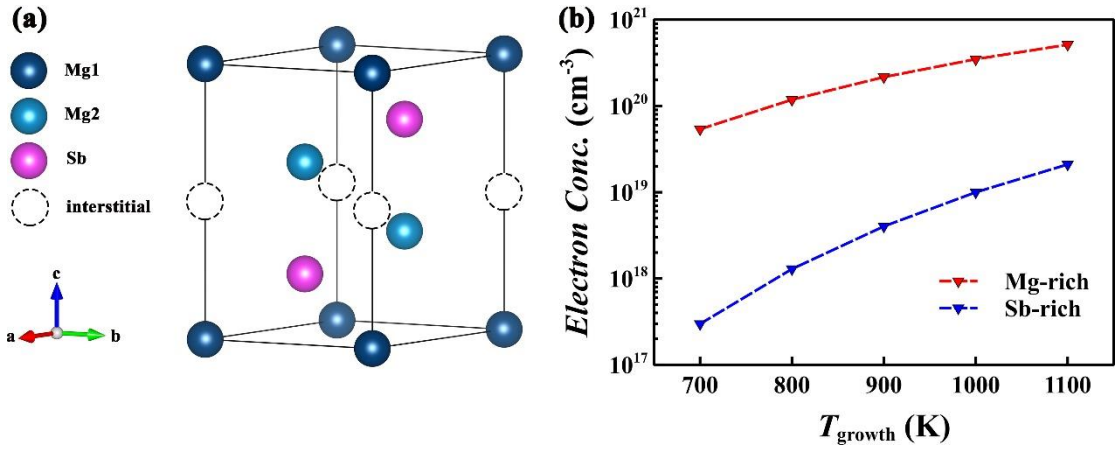

Fig. S2 (a) The crystal structure of Mg_3Sb_2 used for defect calculations. (b) Theoretically calculated electron concentrations for Mg_3Sb_2 doped with Gd under the Mg-rich and Sb-rich conditions.

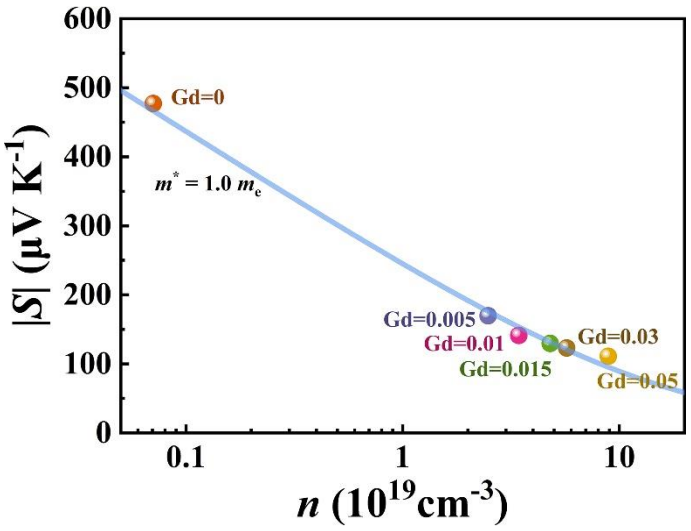

Fig. S3 Room temperature experimental *S vs n* data, in comparison with the Pisarenko plot calculated by using single parabolic band (SPB) model.

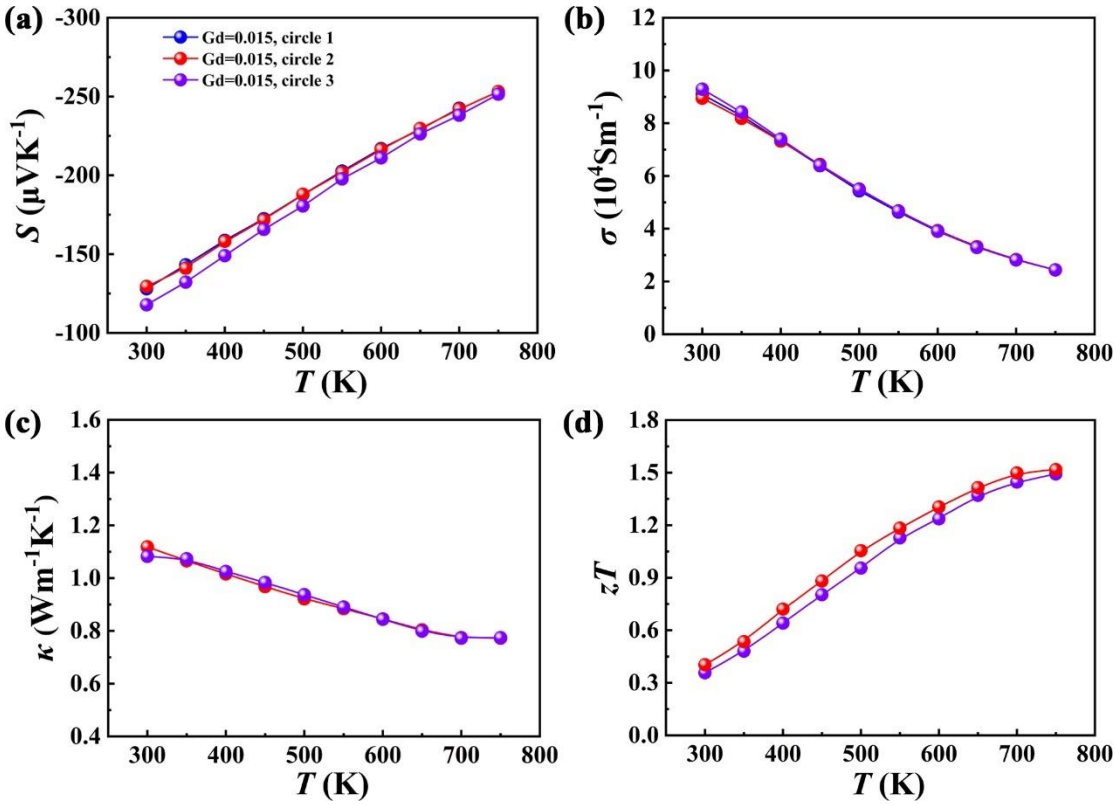

Fig. S4 Reproducible testing of (a) Seebeck coefficient *S*, (b) electrical conductivity *σ*, (c) thermal conductivity *κ*, and (d) *zT* for $Mg_{3.065}Sb_{1.3}Bi_{0.7}Gd_{0.015}$.

Table S1. Parameters used to fit the lattice thermal conductivity (κ_L) for $Mg_{3.065}Sb_{1.3}Bi_{0.7}Gd_{0.015}$.

Fitting Parameters	$Mg_{3.065}Sb_{1.3}Bi_{0.7}Gd_{0.015}$
L (μm)	20
A (10^{-41} s^3)	16.9
B (10^{-18} s K^{-1})	30