

## Supporting Information

# Large improvement in thermoelectric performance of pressure-tuned $\text{Mg}_3\text{Sb}_2$

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## Supplementary Table

**Table S1** The calculated total energy (eV) of  $\text{Mg}_3\text{Sb}_2$  with a series of  $k$ -mesh at different pressure using PBE functional.

$k$ -mesh	2 GPa	4 GPa	8 GPa	10 GPa
10×10×6	-14.6208	-14.5460	-14.3032	-14.1498
12×12×8	-14.6207	-14.5454	-14.3031	-14.1497
16×16×12	-14.6207	-14.5453	-14.3030	-14.1496