

Supporting Information

Large improvement in thermoelectric performance of pressure-tuned Mg_3Sb_2

Juan Li,^{*} Shuai Zhang, Kai Han, Bing Sun and Lianzhen Cao

*Department of Physics and Optoelectronic Engineering, Weifang University, Weifang 261061,
China*

Supplementary Table

Table S1 The calculated total energy (eV) of Mg_3Sb_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