

First-principles study of thermoelectric properties of Mg₂Si- Mg₂Pb semiconductor materials

Tao Fan,^{*ab} Congwei Xie,^{ac} Shiyao Wang,^a Artem R. Oganov^{*acd} and Laifei Cheng^b

^aInternational Center for Materials Discovery, School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, P. R. China. E-mail: nwpufant@mail.nwpu.edu.cn

^bScience and Technology on Thermostructural Composite Materials Laboratory, School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, P. R. China.

^cSkolkovo Innovation Center, Skolkovo Institute of Science and Technology, Moscow 143026, Russia. E-mail: A.Oganov@skoltech.ru

^dMoscow Institute of Physics and Technology, 9 Institutskiy Lane, Dolgoprudny City, Moscow Region 141700, Russia

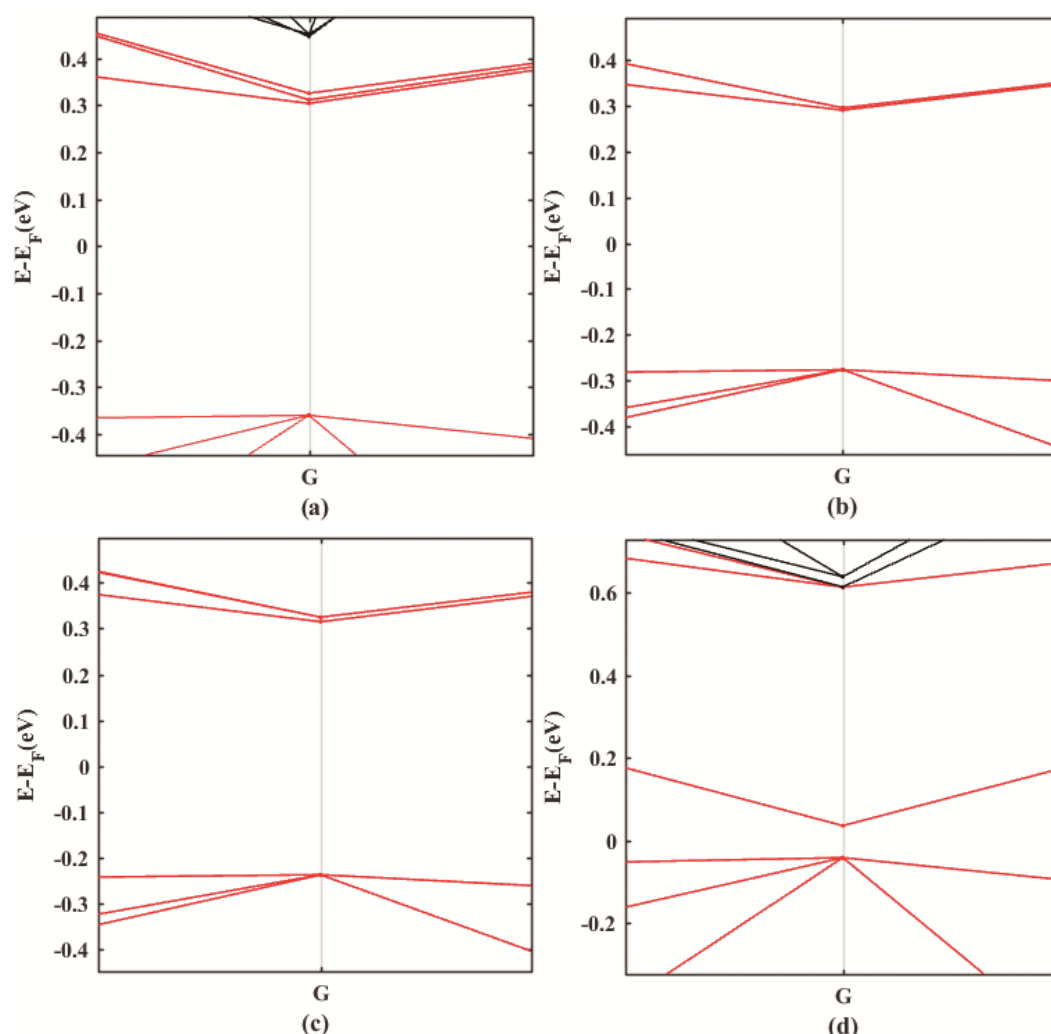


Fig. S1 Enlarged drawings of band structure near band gap. (a) Mg₂Si; (b) Mg₆₄Si₃₁Pb; (c) Mg₆₄Si₃₀Pb₂; (d) Mg₈Si₃Pb. In each figure, the Fermi level E_F was shifted to zero.

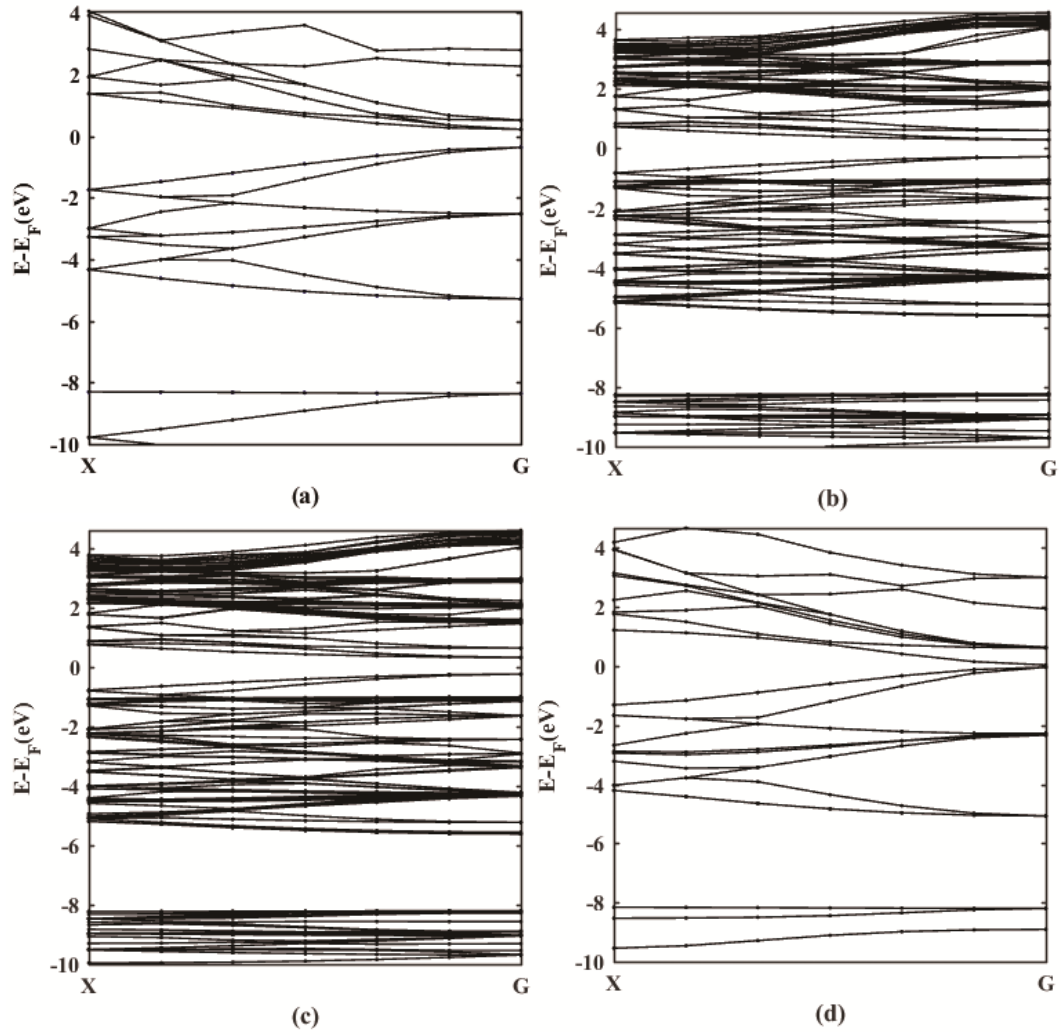


Fig. S2 Band structures along X-G path. (a) Mg_2Si ; (b) $\text{Mg}_{64}\text{Si}_{31}\text{Pb}$; (c) $\text{Mg}_{64}\text{Si}_{30}\text{Pb}_2$; (d) $\text{Mg}_8\text{Si}_3\text{Pb}$. In each figure, the Fermi level E_F was shifted to zero.