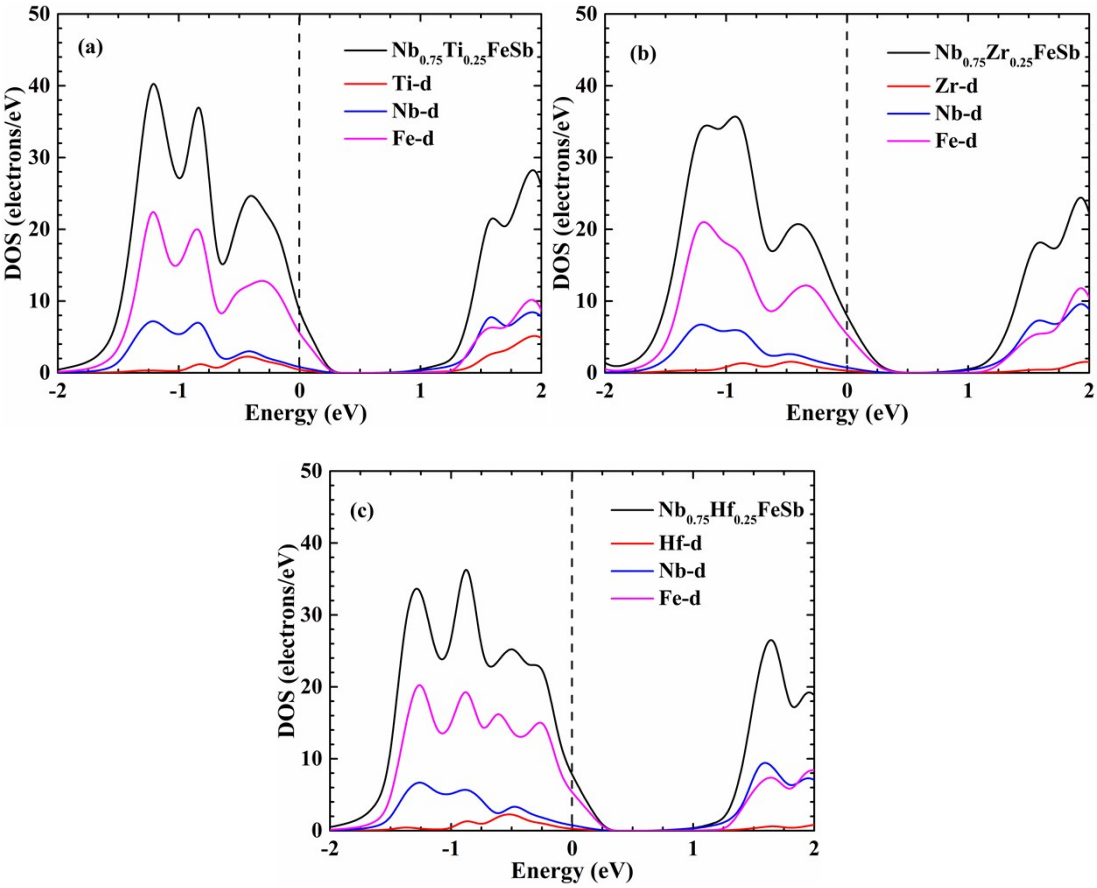
Electronic Supplementary Information

Supplementary Table 1. The calculated lattice constant (a), zero-pressure bulk modulus (B_0) and total energy (E_{tot}) of NbFeSb-based compounds in the conventional cell. The lattice constant (a) and zero-pressure bulk modulus (B_0) were obtained by fitting the calculated total energy-atomic volume (E–V) results to the Murnaghan equation of state (EOS).

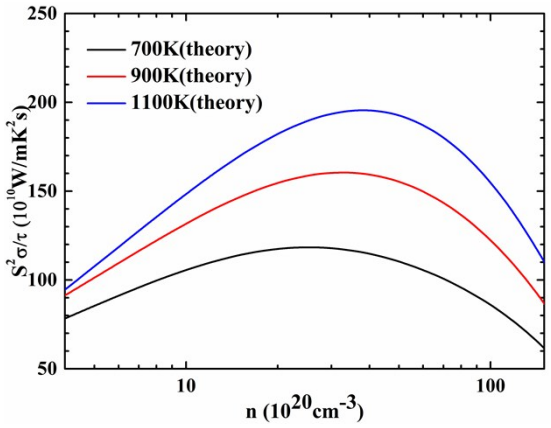
Material	Reference	a (Å)	B_0 (GPa)	E_{tot} (eV)
NbFeSb	This work	5.968	166	-94.28
/	Experimental [1]	5.949	/	/
/	Theory [2]	5.971	161	/
$Nb_{0.75}Ti_{0.25}FeSb$	This work	5.959	/	-92.14
$Nb_{0.76}Ti_{0.24}FeSb$	Experimental [1]	5.939	/	/
$Nb_{0.75}Zr_{0.25}FeSb$	This work	6.009	/	-92.87
$Nb_{0.75}Hf_{0.25}FeSb$	This work	6.000	/	-94.21

Supplementary Table 2. The calculated bulk modulus (B in GPa), shear modulus (G in GPa), shear sound velocity (v_s in m/s), longitudinal sound velocity (v_l in m/s), and the minimum lattice thermal conductivity (κ_{min} in W/mK) of NbFeSb. The calculations were performed by VASP 5.2.

Reference	B	G	v_s	v_l	κ_{min}
This work	163	79	3050	5621	0.96
Theory [2]	158	88	3227	5699	1.00



Supplementary Figure 1. Total DOS of $Nb_{0.75}R_{0.25}FeSb$ (R = Ti, Zr and Hf) and the d-states of R, Nb, Fe atom.



Supplementary Figure 2. Carrier concentration dependence of power factor over relaxation time $S^2\sigma/\tau$ of p-type NbFeSb at 700 K, 900 K and 1100 K.

References

[1] C. G. Fu, T. J. Zhu, Y. T. Liu, H. H. Xie, X. B. Zhao, *Energy Environ. Sci.,* 2015, **8**, 216-220.

[2] C. Çoban, K. Çolakoğlu, Y. Ö. Çiftçi, *Phys. Scr.* 2015, **90**, 095701.