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Supplementary Information

Thermoelectric property enhancement by merging bands in NbFeSb-based half-Heusler mixtures

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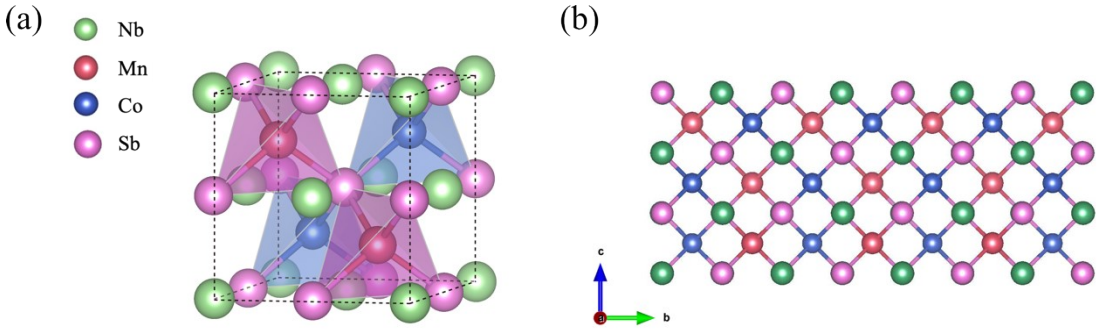

Fig.S1 (a) $Nb_4Mn_2Co_2Sb_4$ local geometry structure, (b) View along the a direction: Mn and Co atoms (or the Mn-Sb and Co-Sb tetrahedrons) are arranged alternately along the b direction.

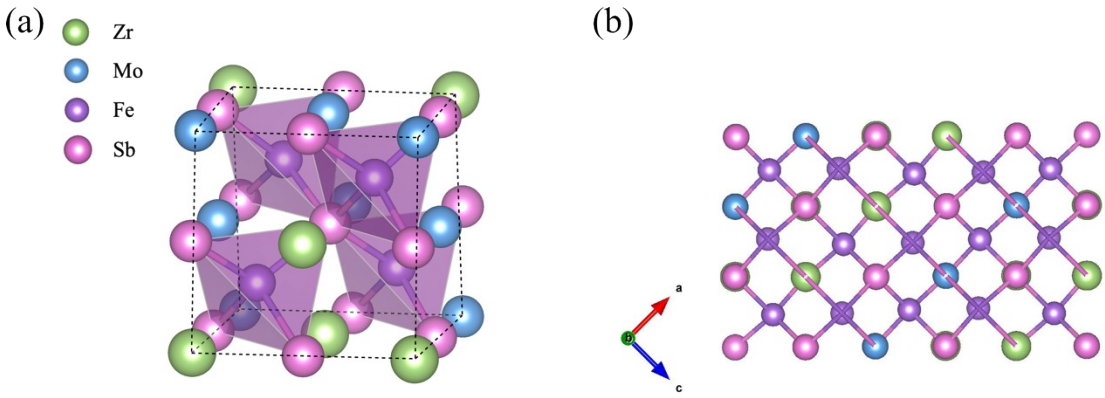

Fig.S2 (a) $Zr_2Mo_2Fe_4Sb_4$ local geometry structures (b) View along the b direction: Zr and Mo atoms are arranged alternately, and form a NaCl-sublattice with Sb atoms, Fe atoms fill the center of the tetrahedral consisting of Fe-Sb.

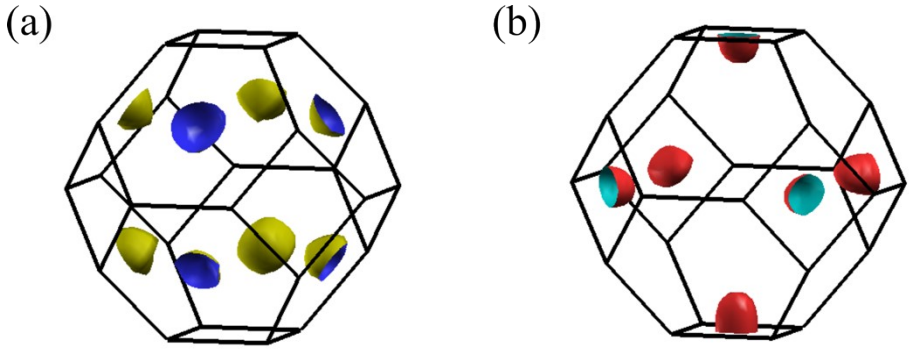

Fig S3 Fermi pockets of NbFeSb at (a) 0.1 eV below the VBM and (b) 0.1 eV above the CBM.

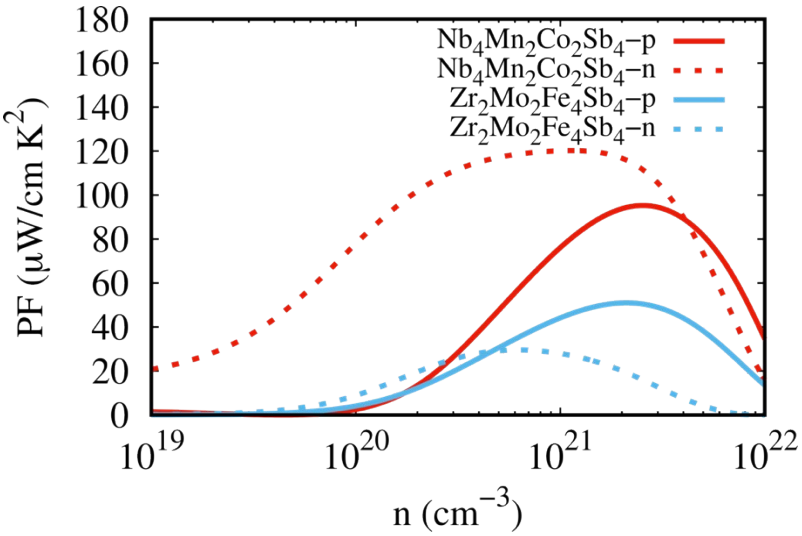

Fig S4 Carrier concentration dependent power factors (PF) of $Nb_4Mn_2Co_2Sb_4$ (red lines) and $Zr_2Mo_2Fe_4Sb_4$ (blue lines) at 900K. The solid and dash lines represent the p- and n-type thermoelectric properties.

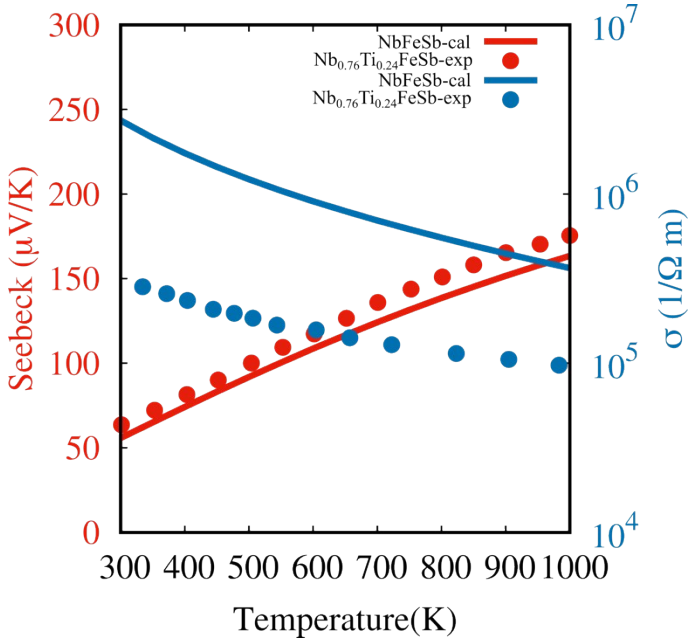

Fig S5 The calculated Seebeck coefficient (the red lines) and electric conductivity (the blue lines) using the deformation potential method. The experimental data (the dotted lines) are taken from Ref [17].

Weighted mobility is defined as:

$$\mu_w = 331\frac{cm^2}{Vs}\left(\frac{m\Omega\ cm}{\rho}\right)\left(\frac{T}{300K}\right)^{-\frac{3}{2}}\left[\frac{\exp\left[\frac{|S|}{k_B/e}-2\right]}{1+\exp\left[-5\left(\frac{|S|}{k_B/e}-1\right)\right]}+\frac{\frac{3}{\pi^2}\frac{|S|}{k_B/e}}{1+\exp\left[5\left(\frac{|S|}{k_B/e}-1\right)\right]}\right] \quad (1)$$

Here, ρ is the electrical resistivity in $m\Omega\ cm$, T is the absolute temperature in K, S is the Seebeck coefficient, and $k_B/e = 86.3\ \mu V\ K^{-1}$.

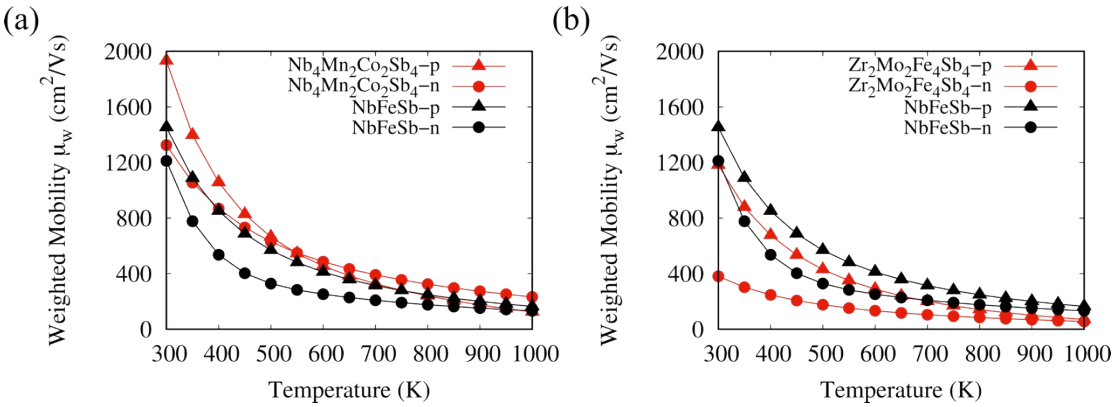

Fig S6 Weighted mobilities of $Nb_4Mn_2Co_2Sb_4$ (the red lines in a) and $Zr_2Mo_2Fe_4Sb_4$ (the red lines in b) compared with NbFeSb (the black lines). The triangle and circle lines represent the p- and n-type thermoelectric properties.