Supporting information

p-type Co interstitial defects in thermoelectric skutterudite $CoSb_3$ due to the breakage of Sb_4-rings

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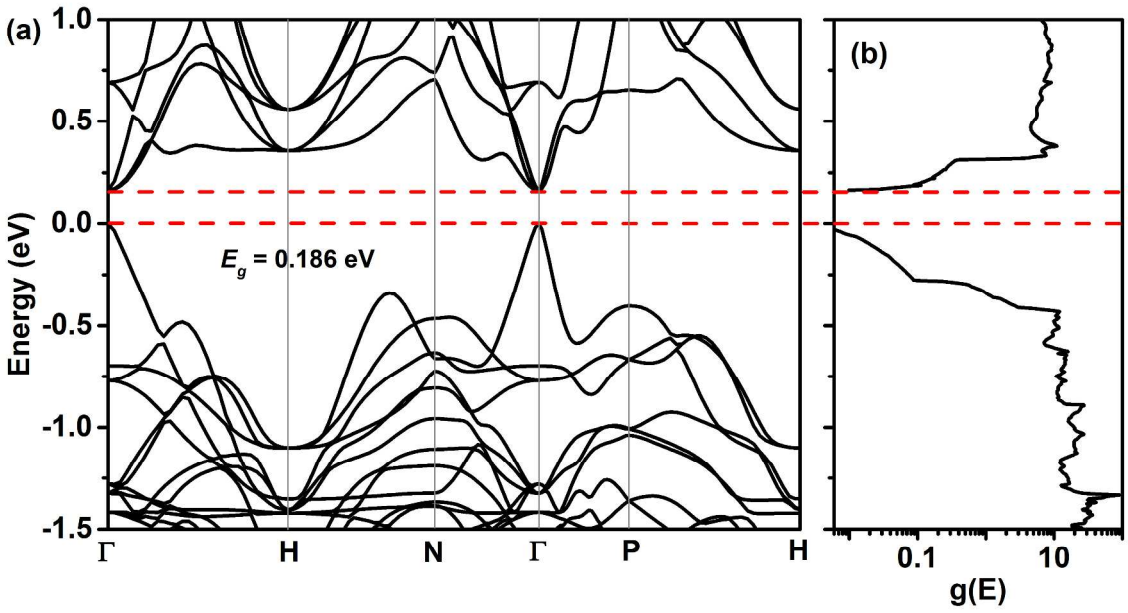

Figure S1. (a) The band structure and (b) density of state of $CoSb_3$ from our *ab-initio* calculation using PBE functional. The direct band gap E_g = 0.186 eV.

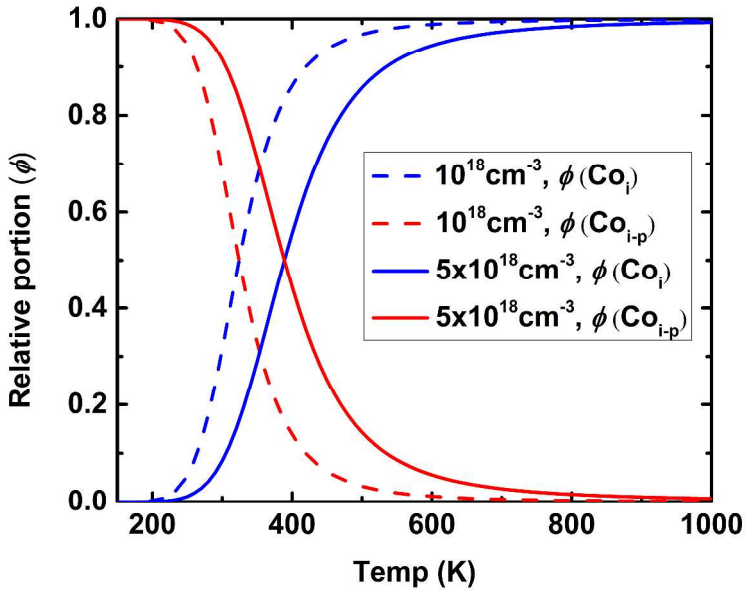

Figure S2. Relative portion of Co_i and $Co_{i\text{-}p}$ as a function of the temperature. Solid line and dot line represent 5×10^{18} cm^{-3} and 10^{18} cm^{-3} carriers in the system respectively. The relation portion is calculated by $\phi=\frac{1}{1+\exp(\frac{\Delta H - T\Delta S}{kT})}$, where ΔH is the formation enthalpy change between neutral Co_i and $Co_{i\text{-}p}$. ΔS is the configurational entropy change defined by equation (3) in the manuscript. The defect thermodynamics calculation is time-independent.