Electronic Supplementary Information

Title

Synergy effect of co-doping Sc and Y in Sb_2Te_3 for phase-change memory

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1. Calculation method for the formation energy of Sc and Y co-doped Sb_2Te_3.

The formation energy for Sc and Y co-doping is calculated as [1]:

$$E^f[X] = E_{\text{tot}}[X] - E_{\text{tot}}[\text{bulk}] - \sum_i n_i \mu_i, \qquad \text{Eq. (S1)}$$

where $E_{\text{tot}}[X]$ and $E_{\text{tot}}[\text{bulk}]$ are the total energies of a supercell with and without Y and Sc doping, respectively, n_i indicates the number of atoms of type *i* (host atoms or impurity atoms) that have been added to ($n_i > 0$) or removed from ($n_i < 0$) the supercell when the doping is created, and μ_i are the corresponding chemical potentials of these species, which can be Te-rich or Te-poor (or anything in between), depending on the experimental growth conditions. The chemical potentials of Sb and Te are related by the following expression: $2\mu_{\text{Sb}} + 3\mu_{\text{Te}} = E_{\text{tot}}[\text{Sb}_2\text{Te}_3]$. Considering the case of the X_2Te_3 compound (X = Sc/Y), the chemical potentials of X and Te are related by the following expression: $2\mu_X + 3\mu_{\text{Te}} = E_{\text{tot}}[X_2\text{Te}_3]$. Under the extreme Te-rich condition, the chemical potential of Te is subject to an upper bound, $\mu_{\text{Te}}^{max} = \mu_{\text{Te}}[\text{bulk}]$. The upper limit on μ_{Te}^{max} then results in lower limits on μ_{Sb} and μ_X:

$$\mu_{\text{Sb}}^{\text{min}} = \left(E_{\text{tot}}[\text{Sb}_2\text{Te}_3] - 3\mu_{\text{Te}}[\text{bulk}]\right)/2 \qquad \text{Eq. (S2)}$$

$$\mu_X^{\text{min}} = \left(E_{\text{tot}}[X_2\text{Te}_3] - 3\mu_{\text{Te}}[\text{bulk}]\right)/2. \qquad \text{Eq. (S3)}$$

Similarly, under the extreme Te-poor condition, the chemical potential of Te is subject to a lower limit:

$$\mu_{\text{Te}}^{\text{min}} = \max\begin{cases}\left(\text{E}_{\text{tot}}[\text{Sb}_2\text{Te}_3] - 2\mu_{Sb}[\text{bulk}]\right)/3 \\ \left(\text{E}_{\text{tot}}[X_2\text{Te}_3] - 2\mu_X[\text{bulk}]\right)/3\end{cases} \qquad \text{Eq. (S4)}$$

which results in upper limits on μ_{Sb} and μ_X:

$$\mu_{\text{Sb}}^{\text{max}} = \left(E_{\text{tot}}[\text{Sb}_2\text{Te}_3] - 3\mu_{\text{Te}}^{\text{min}}\right)/2 \qquad \text{Eq. (S5)}$$

$$\mu_X^{\text{max}} = \left(E_{\text{tot}}[X_2\text{Te}_3] - 3\mu_{\text{Te}}^{\text{min}}\right)/2 \qquad \text{Eq. (S6)}$$

In our calculations, the trigonal phase of Sb and Te, and the hexagonal phases of Y/Sc were used as the reference elemental bulk phases for the chemical potentials.

The $E_{tot}[Sb_2Te_3]$ and $E_{tot}[X_2Te_3]$ values in Eq. (A.2-6) are the total energies of the primitive cell of Sb_2Te_3 and X_2Te_3 (X = Sc/Y), respectively.

2. Doping modes and optimal configurations of Sc and Y co-doping Sb_2Te_3.

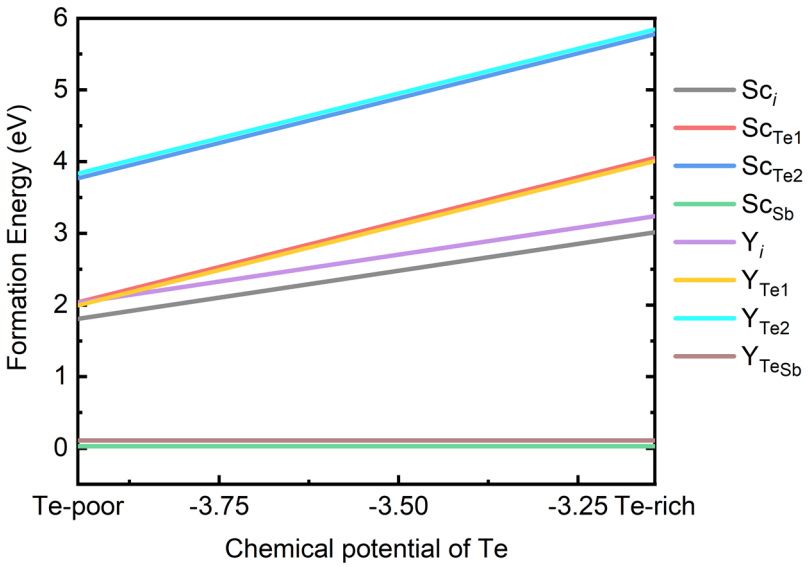

Figure S1. The calculated formation energies for Sc and Y occupying various positions, referred to as X_{Sb}, X_{Te1}, X_{Te2} and X_i in Sb_2Te_3 (X = Sc/Y).

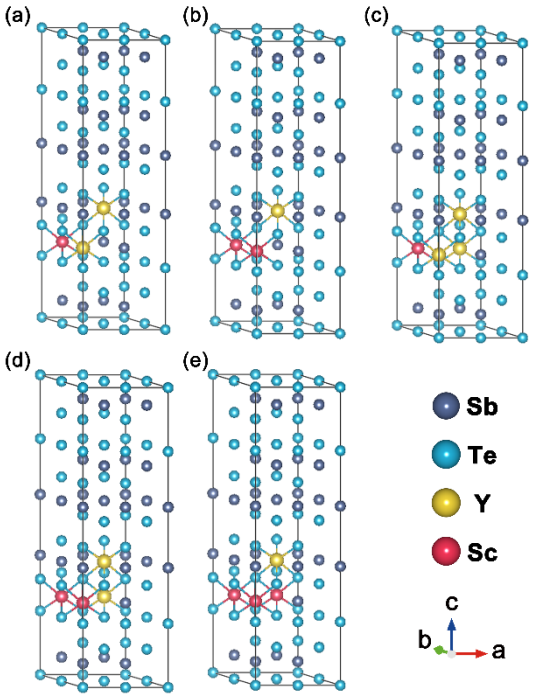

Figure S2. The configurations with the lowest total energy for $Sc_{x_1}Y_{x_2}Sb_{2-x_1-x_2}Te_3$, where: (a) x_1=0.083, x_2=0.167; (b) x_1=0.167, x_2=0.083; (c) x_1=0.083, x_2=0.250; (d) x_1=0.167, x_2=0.167; (e) x_1=0.250, x_2=0.083.