**Supplementary Information**

# The Effect of Na and Ag Doping – Alone and in Combination – on $SnS_{1-x}Se_x$ Nanostructured Thermoelectric Materials

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**Table S1.** Average particle sizes and mean crystalline sizes

| Sample | Type | Average particle size (nm) | Mean crystalline size (nm) |
|---|---|---|---|
| **SnS** | NPs | 28.9 ± 8.1 | 19.0 |
| | Pellet | N/A | 36.0 |
| **SnS:Na** | NPs | 26.9 ± 6.7 | 23.4 |
| | Pellet | N/A | 39.2 |
| **$SnS_{0.9}Se_{0.1}$:Na** | NPs | 23.2 ± 6.0 | 19.8 |
| | Pellet | N/A | 36.0 |
| **$SnS_{0.9}Se_{0.1}$:Ag** | NPs | 21.2 ± 5.8 | 8.5 |
| | Pellet | N/A | 39.2 |
| **$SnS_{0.9}Se_{0.1}$:Na,Ag** | NPs | 21.3± 5.9 | 10.6 |
| | Pellet | N/A | 36.0 |

The average particle size was determined from TEM images, and the mean crystalline size was estimated from the XRD peaks of the NPs.

**Table S2.** Compositions of the NPs measured by SEM-EDS

| NPs | Sn (at%) | S (at%) | Se (at%) | Ag (at%) |
|---|---|---|---|---|
| **SnS** | 51.9 | 48.1 | N/A | N/A |
| **SnS:Na** | 51.5 | 48.5 | N/A | N/A |
| **$SnS_{0.9}Se_{0.1}$:Na** | 51.6 | 42.4 | 6.0 | N/A |
| **$SnS_{0.9}Se_{0.1}$:Ag** | 52.1 | 41.9 | 4.5 | 1.5 |
| **$SnS_{0.9}Se_{0.1}$:Na,Ag** | 53.2 | 40.5 | 5.0 | 1.3 |

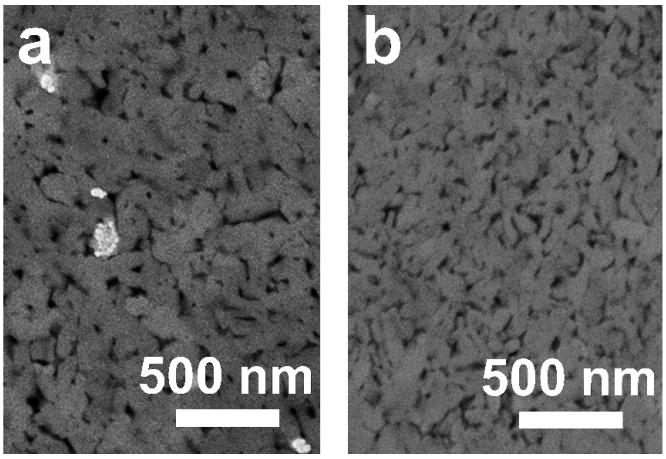


**Figure S1.** Enlarged versions of the higher magnification insets of the SEM images given in Fig. 3, for the (a) $SnS_{0.9}Se_{0.1}$:Ag and (b) $SnS_{0.9}Se_{0.1}$:Na,Ag pellets.

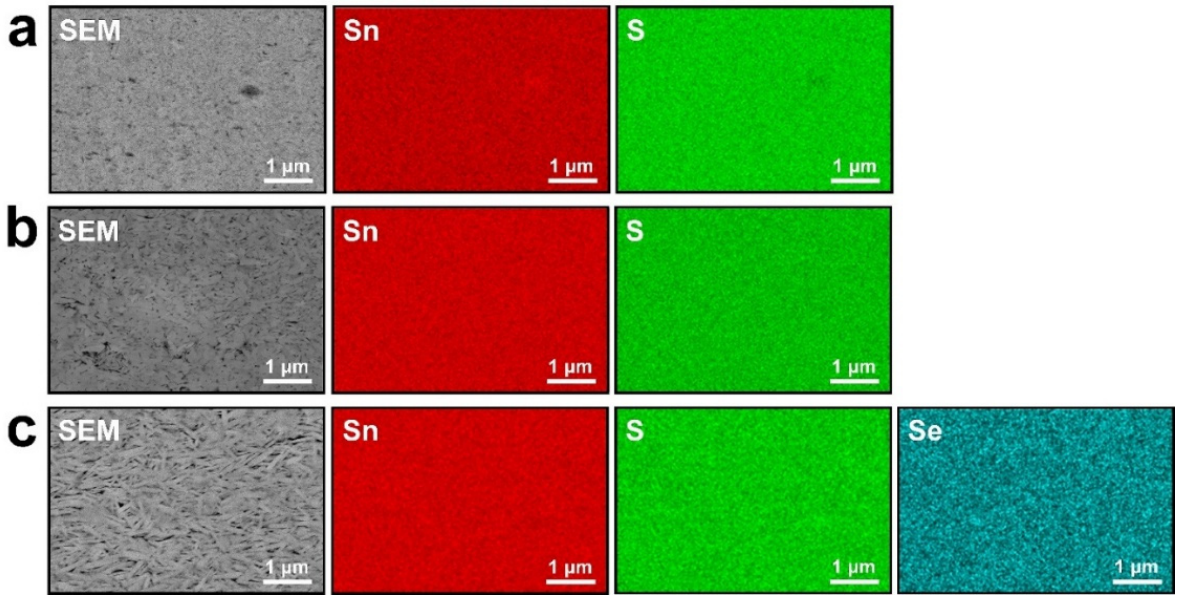


**Figure S2.** SEM images and corresponding EDS elemental maps of pellets of (a) SnS, (b) SnS:Na and (c) $SnS_{0.9}Se_{0.1}$:Na. The leftmost grayscale images are SEM images. Red, green and blue images are EDS elemental maps for Sn, S and Se, respectively.

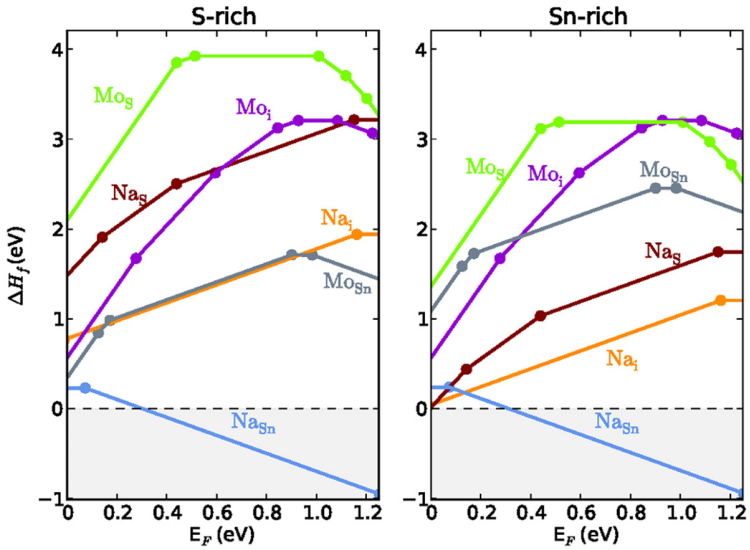


**Figure S3.** Calculated defect formation enthalpies for extrinsic defects formed from the elements Na and Mo, under S-rich (left) and Sn-rich (right) conditions. Reproduced from ref. 47 with permission from the Royal Society of Chemistry.

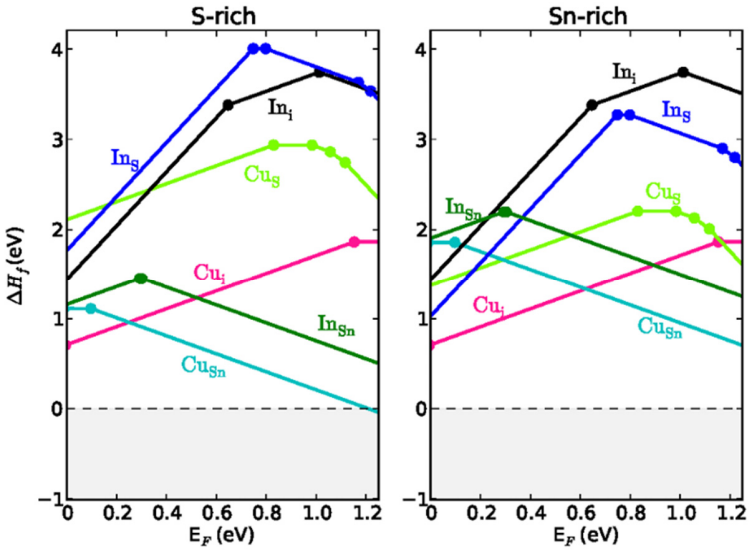


**Figure S4.** Calculated defect formation enthalpies for extrinsic defects formed from the elements Cu and In, under S-rich (left) and Sn-rich (right) conditions. Reproduced from ref. 47 with permission from the Royal Society of Chemistry.