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CORRECTION

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Correction: Significant average *ZT* enhancement in Cu_3SbSe_4-based thermoelectric material *via* softening p–d hybridization

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Correction for 'Significant average *ZT* enhancement in Cu_3SbSe_4-based thermoelectric material *via* softening p–d hybridization' by Dan Zhang *et al.*, *J. Mater. Chem. A*, 2019, DOI: 10.1039/c9ta05115e.

The authors regret the following errors in the labelling of Cu and Ag orbitals in the published article:

In the Results and discussion section, the text "The calculated partial density of states (PDOS) for pristine Cu_3SbSe_4 (Fig. S3†) shows the valence band is dominated by strong hybridization between Cu 4d orbitals and Se 4p orbitals, whereas the conduction band edge is mainly formed of Sb 5s orbitals and p orbitals of neighboring Se. As Ag 5d orbitals are located at much lower energies (Fig. 4e)…" should instead read as follows: "The calculated partial density of states (PDOS) for pristine Cu_3SbSe_4 (Fig. S3†) shows the valence band is dominated by strong hybridization between Cu 3d orbitals and Se 4p orbitals, whereas the conduction band edge is mainly formed of Sb 5s orbitals and p orbitals of neighboring Se. As Ag 4d orbitals are located at much lower energies (Fig. 4e)…"

In Fig. 4e, the labels 'Cu 4d' and 'Ag 5d' should instead read 'Cu 3d' and 'Ag 4d', respectively. A corrected version of Fig. 4 is provided below.

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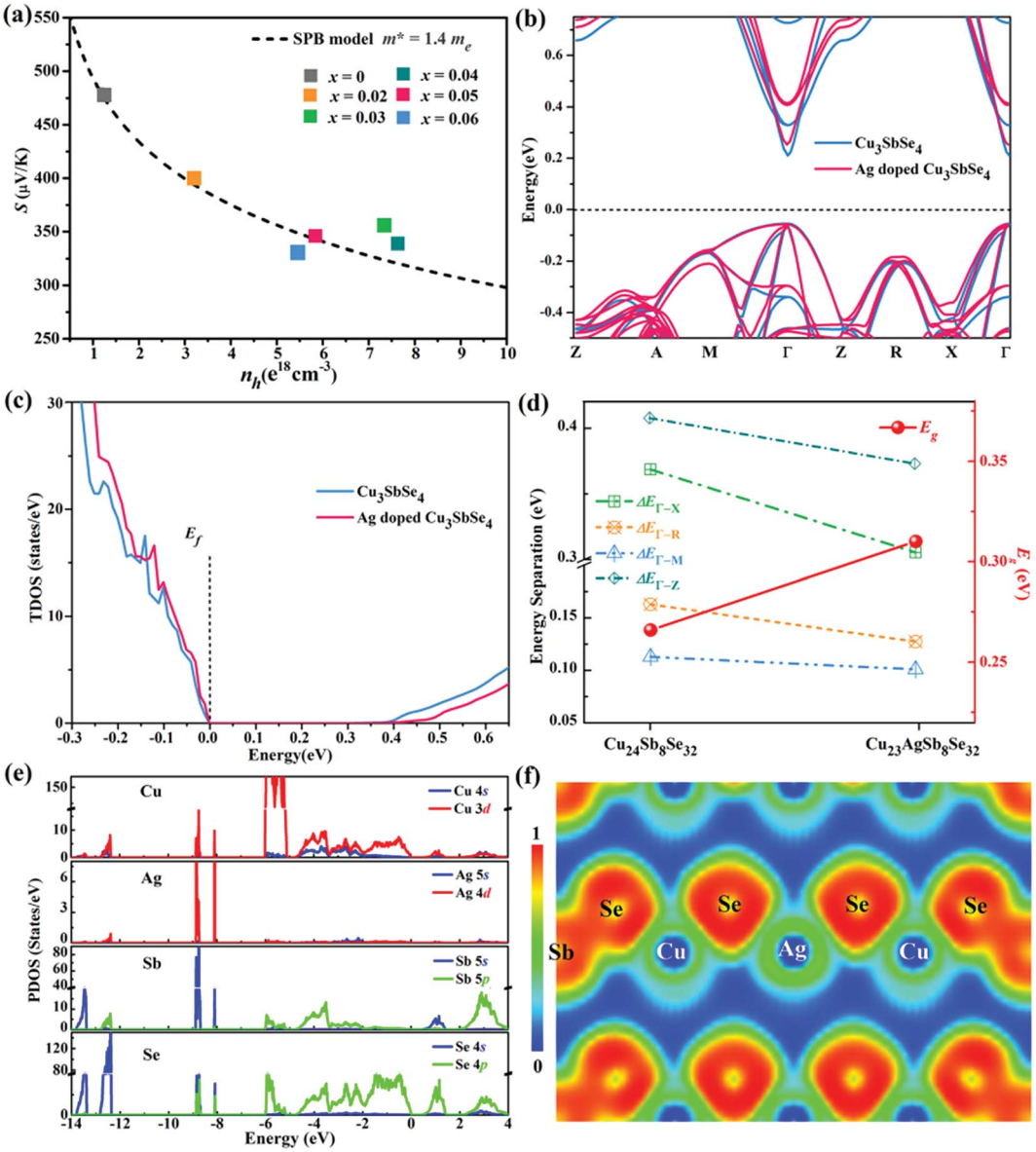

Fig. 4 (a) The change of Seebeck coefficient *versus* hole concentration at room temperature (*i.e.* Pisarenko curve). (b and c) Calculated band structure and total density of states (TDOS) for pristine Cu_3SbSe_4 and Ag-doped Cu_3SbSe_4. (d) Determined band gap E_g, and the energy difference ΔE of the first valence band between different high asymmetry point and gamma point from the calculated band structure. (e) Partial density of states (PDOS) of Ag-doped Cu_3SbSe_4. (f) The calculated ELF of Ag-doped Cu_3SbSe_4 (101) surface in which Ag–Se atoms have less overlapped electrons compared with Cu–Se; the respective bond lengths of Ag–Se and Cu–Se are 2.67999 and 2.41058 Å.

In the originally published version of Fig. S3, the label 'Cu 4d' should instead have read 'Cu 3d'. This error has now been corrected in the ESI which is available online.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.