

## Electronic Supplementary Information

### High thermoelectric performance of Ag doped SnTe polycrystalline bulks via the synergistic manipulation of electrical and thermal transport

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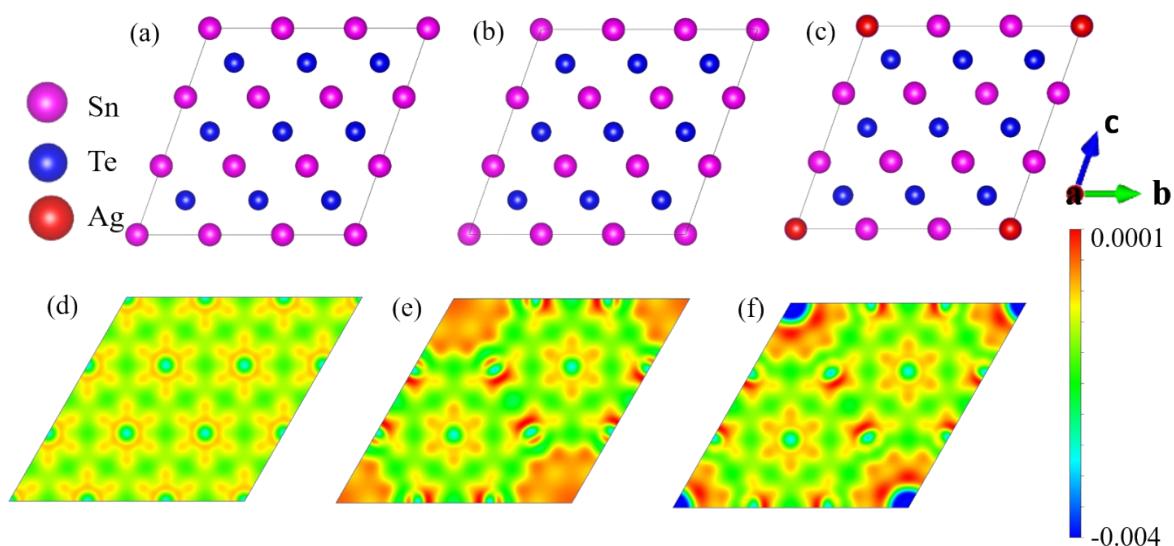


Fig. S1  $\text{Sn}_{27}\text{Te}_{27}$  (a),  $\text{Sn}_{26}\text{Te}_{27}$  (b), and  $\text{Sn}_{26}\text{AgTe}_{27}$  (c) primitive cells used for the DFT calculations, and the 2-dimensional charge density difference for the (001) planes of  $\text{Sn}_{27}\text{Te}_{27}$  (d),  $\text{Sn}_{26}\text{Te}_{27}$  (e), and  $\text{Sn}_{26}\text{AgTe}_{27}$  (f). Blue and yellow colours represent loss and gain of electrons, respectively.

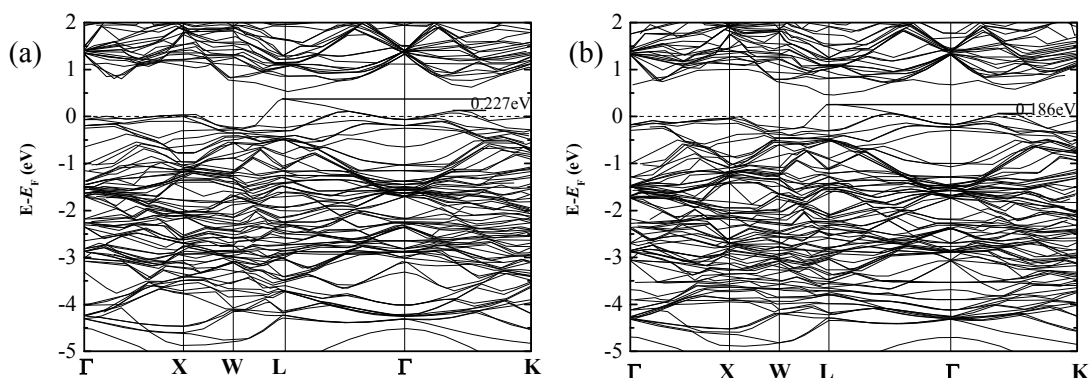


Fig. S2 Calculated electronic band structures for the Sn-deficient  $\text{Sn}_{26}\text{Te}_{27}$  (a) and silver-doped  $\text{Sn}_{26}\text{AgTe}_{27}$  (b) using Perdue Burke Ernzerhof generalized gradient approximations (PBE-GGA) based on density functional theory (DFT).

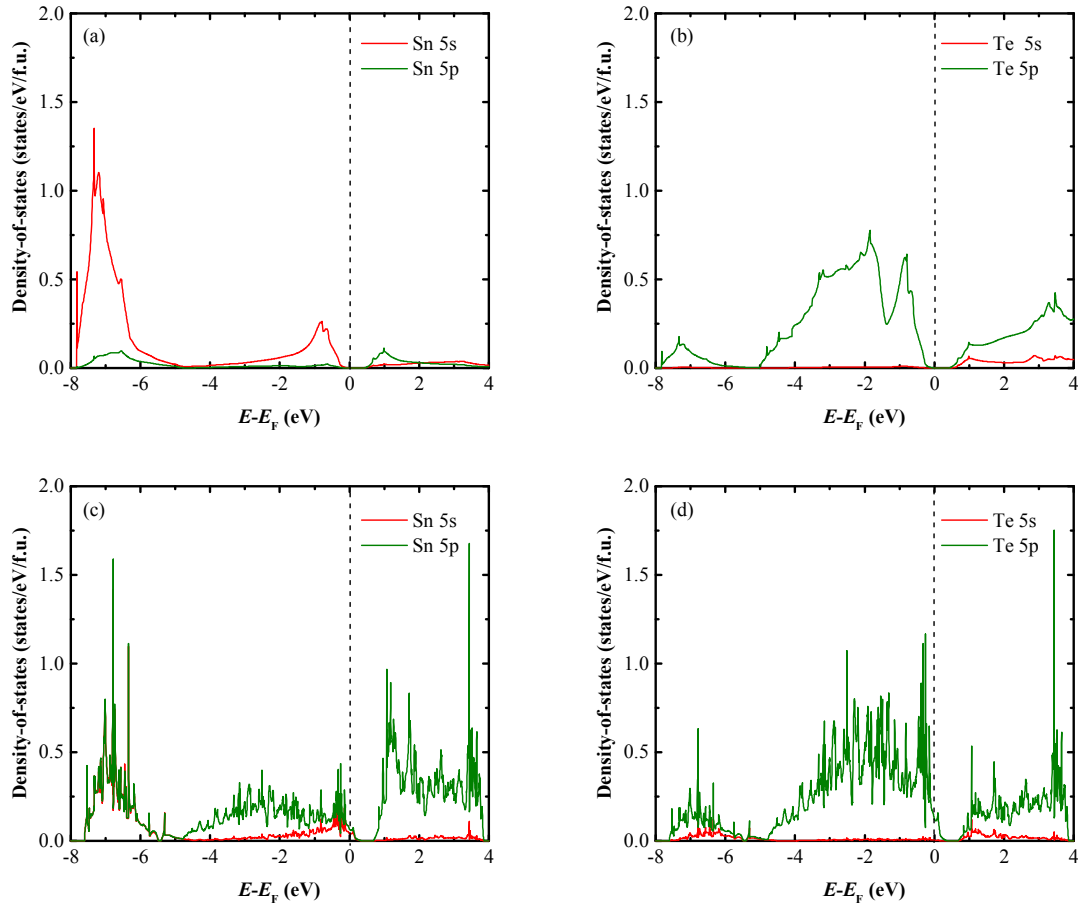


Fig. S3 Calculated partial electronic density-of-states (DOS) for SnTe (a, b) and  $\text{Sn}_{26}\text{Te}_{27}$  (c, d) based on the DFT method.

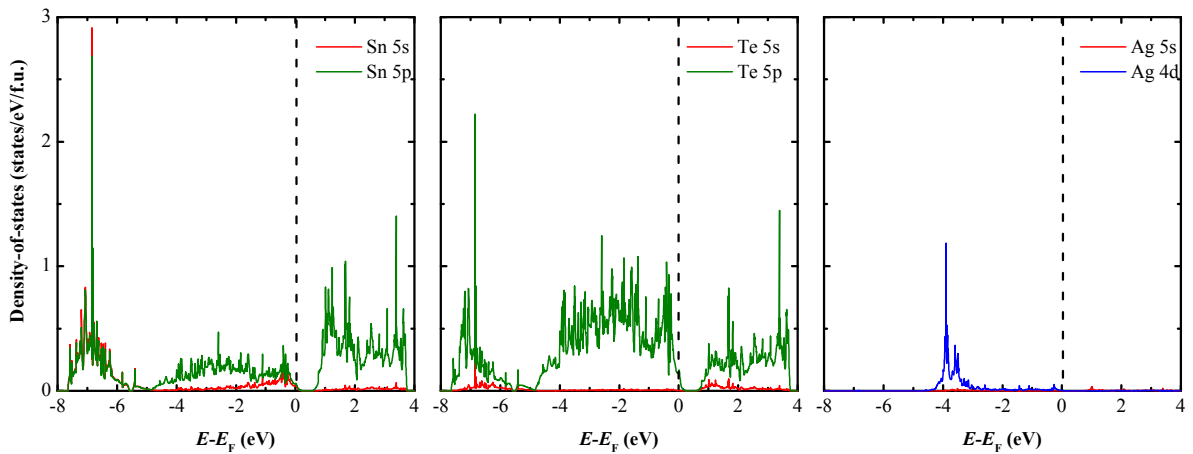


Fig. S4 Calculated partial electronic density-of-states (DOS) for the silver doped  $\text{Sn}_{26}\text{AgTe}_{27}$  based on the DFT method.

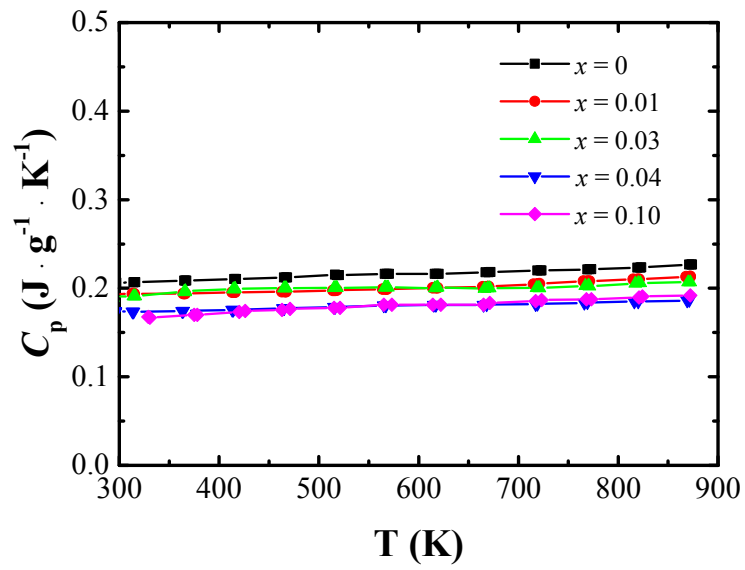


Fig. S5 Temperature dependence of the specific heat for the excess-silver-doped  $\text{SnAg}_x\text{Te}$  ( $x = 0, 0.01, 0.03, 0.04, 0.10$ ) samples.

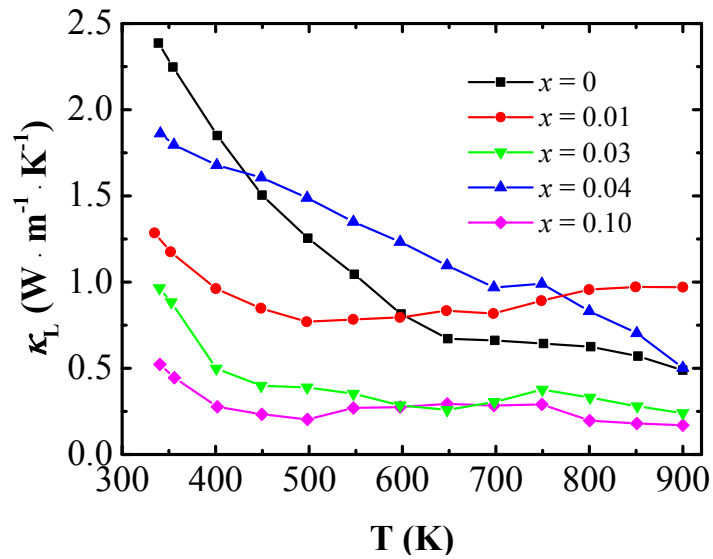


Fig. S6 Temperature dependence of the lattice thermal conductivity ( $\kappa_L$ ) for the synthesized  $\text{SnAg}_x\text{Te}$  ( $x = 0, 0.01, 0.03, 0.04, 0.10$ ) samples.