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

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

Fig. S2 Calculated electronic band structures for the Sn-deficient Sn_{26}Te_{27} (a) and silver-doped Sn_{26}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 Sn$_{26}$Te$_{27}$ (c, d) based on the DFT method.

Fig. S4 Calculated partial electronic density-of-states (DOS) for the silver doped Sn$_{26}$AgTe$_{27}$ based on the DFT method.
Fig. S5 Temperature dependence of the specific heat for the excess-silver-doped SnAg$_x$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 SnAg$_x$Te ($x = 0, 0.01, 0.03, 0.04, 0.10$) samples.