Electronic Supplementary Material (ESI) for RSC Advances.

Bi_2Te_3 single crystals with high room-temperature thermoelectric performance enhanced by manipulating point defects based on first-principles calculation

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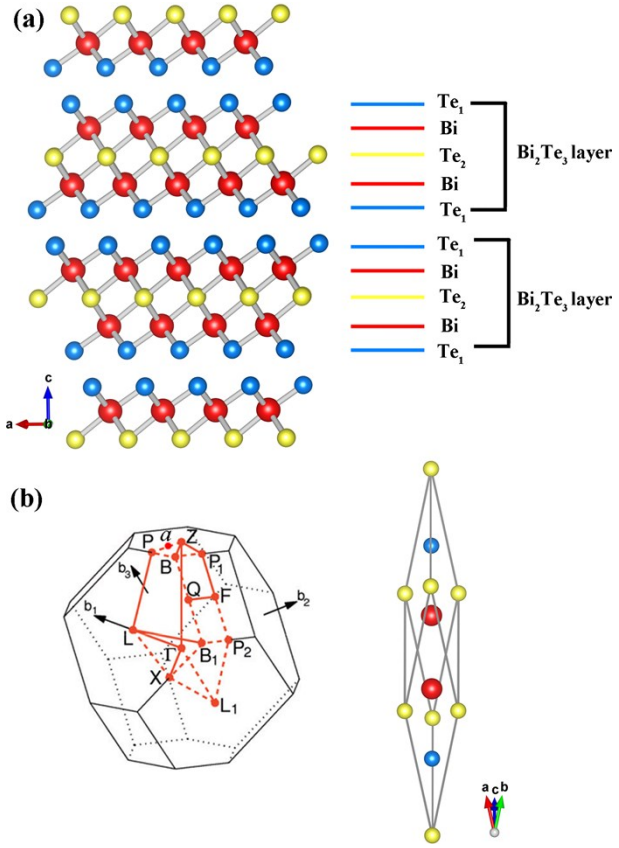

Fig. S1 (a) lamella structure, (b) first Brillouin zone, and (c) primitive unit cell of Bi_2Te_3.

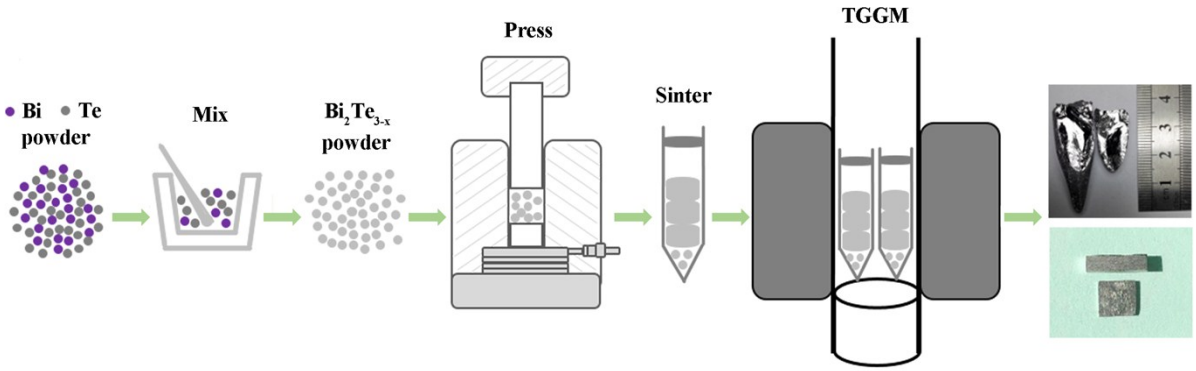

Fig. S2 Schematic illustration of the synthesis procedure for Bi_2Te_{3-x} (x = 0, 0.02, 0.04, 0.06, 0.08) single crystals by the TGGM.

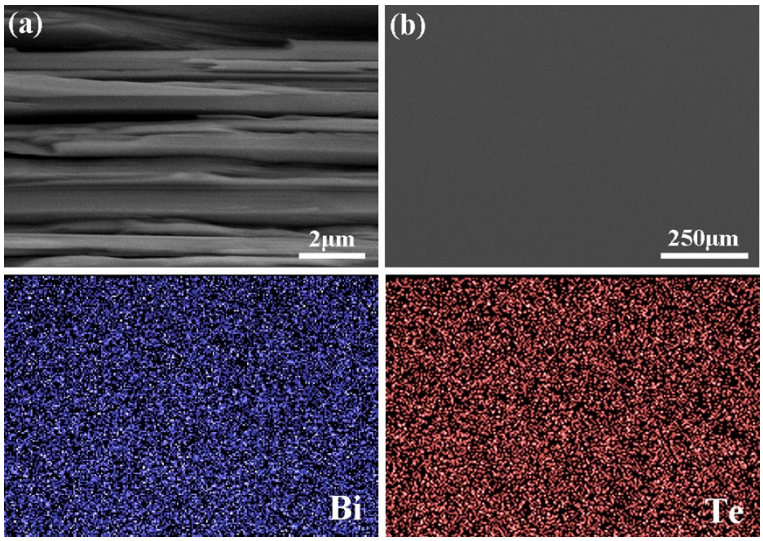

Fig. S3 FESEM images and EDS mapping of Bi and Te elements for x = 0 bulk.

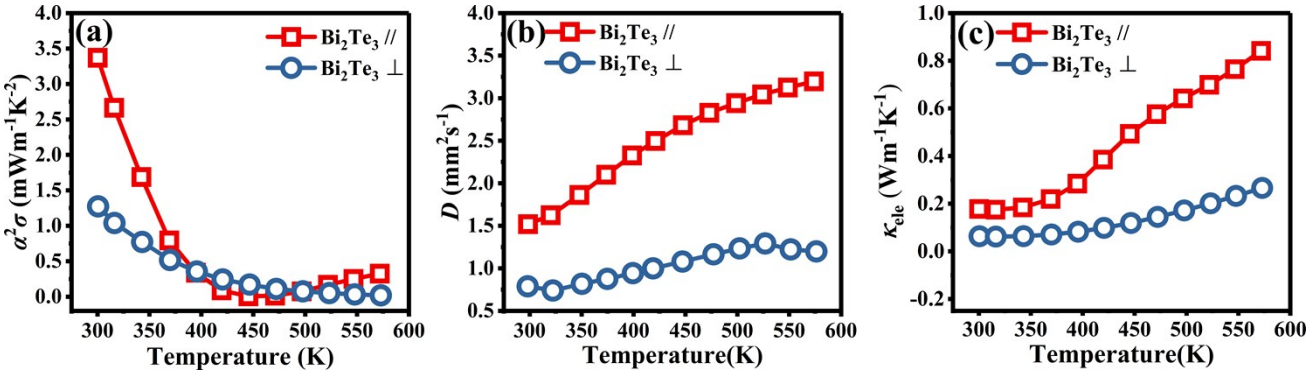

Fig. S4 Temperature dependence of TE properties along the in-plane (//) and out-plane (⊥) for x = 0 bulk. (a) power factor ($\alpha^2\sigma$), (b) thermal diffusivity (D), and (c) electronic thermal conductivity (κ_{ele}).