Electronic Supplementary Material (ESI)

Medium-temperature thermoelectric GeTe: vacancy suppression and band structure engineering leading to high performance

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Fig. S1 Hole carrier concentration dependence of mobility at room temperature.
Fig. S2 (a) PXRD pattern of Bi$_y$Ge$_{1.04-y}$Te. (b) enlarged XRD peaks between 42 – 44° and relationship between content of Bi and angle. (c) enlarged XRD peaks between 61 – 63° and the Bi content dependence of lattice parameter.
Fig. S3 (a) Polished surface morphologies of Bi$_{0.05}$Ge$_{0.99}$Te. (b) Ge (c) Te and (d) Bi mapping.
Fig.S4 Temperature dependent of Hall mobility for Bi$_{1.04-y}$Ge$_y$Te.
Fig. S5 Band structure of (a) pure rhombohedral GeTe (b) Bi doped rhombohedral GeTe (a 2x2x2 supercell was applied and one Ge atom was replaced by one Bi atom).
Fig. S6 Band structure of (a) rhombohedral GeTe (b) cubic GeTe.
Fig. S7 Repeat measurement of (a) electrical resistivity, (b) Seebeck coefficient and (c) thermal conductivity of Ge$_{1.04}$Te.
Fig S8 Repeat measurement of (a) electrical resistivity, (b) Seebeck coefficient, (c) thermal conductivity and (d) calculated ZT value of Bi$_{0.05}$Ge$_{0.99}$Te.