Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

-SUPPLEMENTARY INFORMATION-

The variation of intrinsic defects in XTe (X=Ge, Sn, and Pb) induced by the energy positions of valence band maxima

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The chemical potential of the element determines the growth environment of the crystal. The chemical potential of the element in the XTe system can be defined as:

$$\Delta\mu_X = \mu_X - \mu_X^0 \qquad \Delta\mu_{Te} = \mu_{Te} - \mu_{Te}^0$$

At the same time, it must meet:

(1) The compound can exist stably:

$$\Delta\mu_{X+}\Delta\mu_{Te=}\Delta H_f^{XTe}$$

(2) All component elements should be beneficial to the formation of compounds, not pure phase elements:

$$\Delta\mu_X < 0 \qquad \Delta\mu_{Te} < 0$$

(3) It also requires no second phase impurities, e.g., in PbTe:

$$3\Delta\mu_{Pb+}\Delta\mu_{Te} < \Delta H_f^{Pb_3Te}$$

Among them, μ_X^0 is the chemical potential of metal Ge, Sn and Pb respectively, μ_{Te}^0 is the chemical potential of metal Te, and ΔH_f^{XTe} is the enthalpy of formation of XTe. The energies and enthalpies of all second phases compounds based on Materials Informatics Platform[1]. Figure S1 is the chemical potential range of XTe compounds.

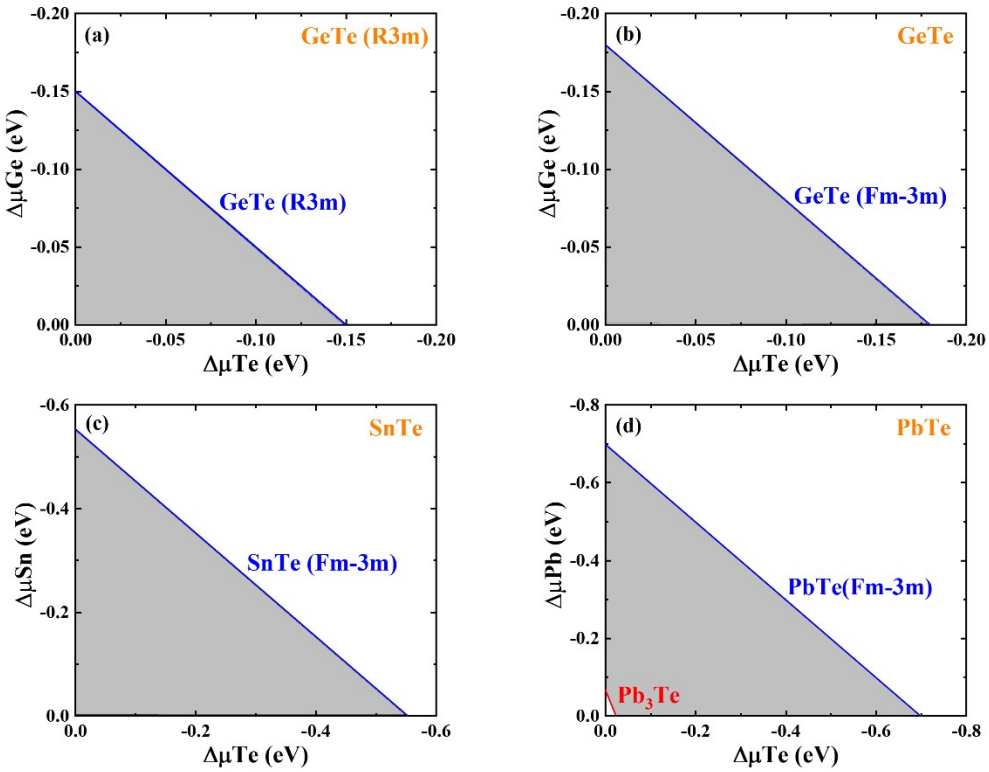

Fig. S1 Chemical potential range of the XTe compounds.(a) (b) (c) (d) are the chemical potential range of GeTe (R3m), GeTe, SnTe, PbTe, respectively.

Table S1 The main intrinsic defects of XTe compounds and formation energy (E_f=0)

Compounds	**GeTe(R3m)**		**GeTe**		**SnTe**		**PbTe**	
	Ge-rich	Ge-poor	Ge-rich	Ge-poor	Sn-rich	Sn-poor	Pb-rich	Pb-poor
$\Delta H_{D,\ q}$ **(eV)**	V_{Ge}^{2-} (-0.35)	V_{Ge}^{2-} (-0.51)	V_{Ge}^{2-} (-0.13)	V_{Ge}^{2-} (-0.32)	V_{Sn}^{2-} (0.18)	V_{Sn}^{2-} (-0.37)	V_{Te}^{2+} (0.05)	Te_{Pb}^{2+} (0.15)
	Te_{Ge}^{2+} (0.22)	Te_{Ge}^{2+} (-0.09)	Ge_{Te}^{2-} (1.12)	Te_{Ge}^{2+} (0.71)	Sn_{Te}^{2-} (0.80)	Te_{Sn} (1.32)	Pb_{Te}^{2+} (0.50)	V_{Pb}^{2-} (0.59)
	Ge_{Te}^{2-} (0.53)	Ge_{Te}^{2+} (0.84)	Te_{Ge}^{2+} (0.93)	Ge_{Te}^{2-} (1.33)	V_{Te}^{2+} (1.473)	Sn_{Te}^{2-} (1.91)	Pb_i^{2+} (0.69)	V_{Te}^{2+} (0.72)

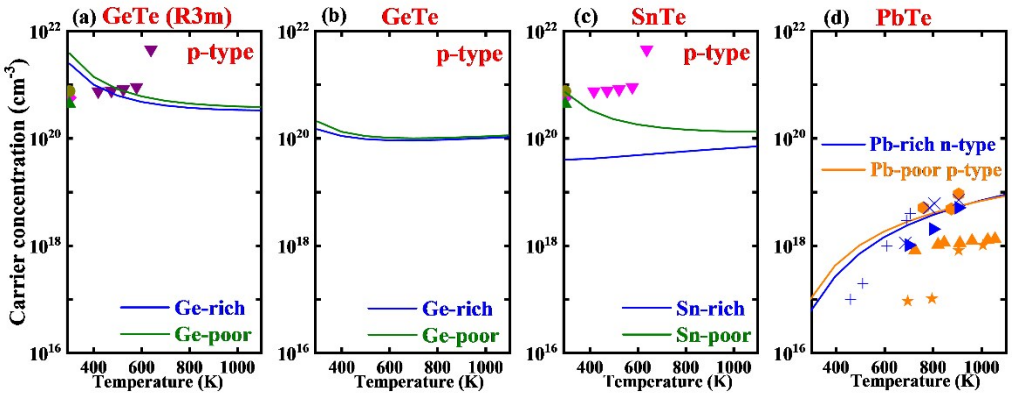

Fig. S2 Under electrically neutral conditions, calculate the relationship between the carrier concentration and temperature in XTe system. (a) Refs.[2-4]; (c) Refs.[5-7]; (d) Refs.[8-11]

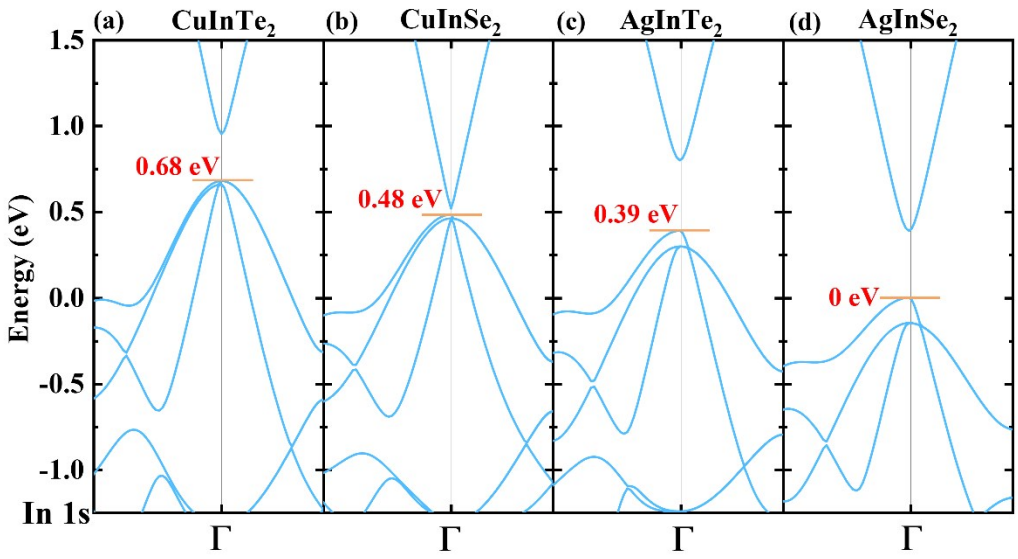

Fig. S3 The aligned bands of 1:1:2 diamond-like system ($CuInTe_2$, $CuInSe_2$, $AgInTe_2$, $AgInSe_2$) based on the In 1s orbitals are shown in (a), (b), (c), (d).

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