Electronic Supplementary Information: The importance of phase equilibrium for doping efficiency: iodine doped PbTe

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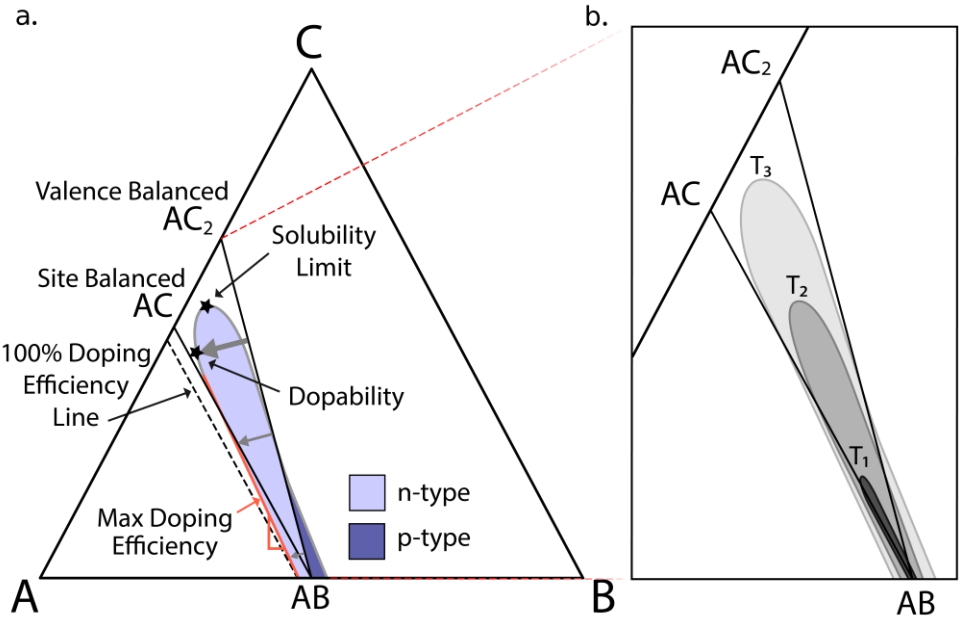

Fig. S1. (a) Schematic, isothermal, ternary phase diagram of a binary semiconductor, AB, doped with C demonstrating various doping concepts (recreated from main text fig. 1). (b) Schematic single-phase region in the same system at three arbitrary temperatures: T_1, T_2, and T_3. The shape of the single-phase region and corresponding doping properties will depend on the thermodynamic state at a given temperature.

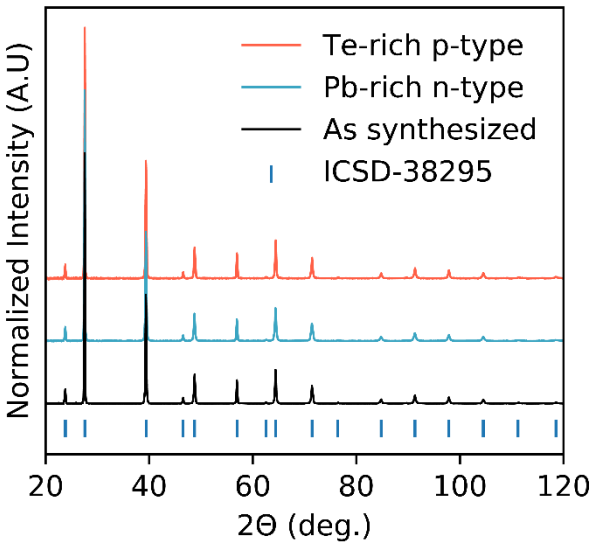

Fig. S2. Example XRD pattern taken on nominally $PbTe_{0.99}I_{0.02}$ samples before and after saturating to Te-rich and Pb-rich compositions showing no observable impurities. The switch between Pb- and Te-rich is accompanied by a switch in conduction from n- to p-type.

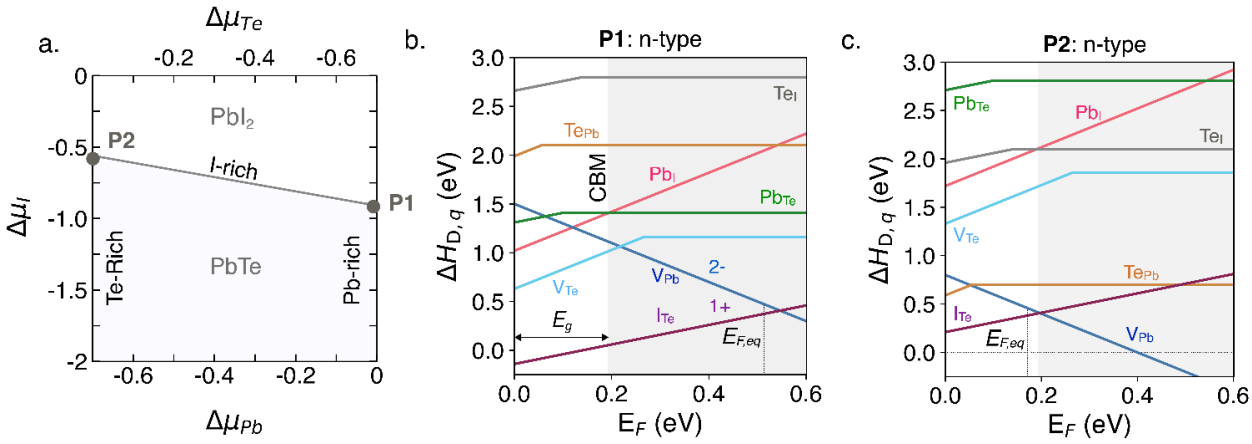

Fig. S3. (a) Phase stability (shaded) of PbTe in the Pb-Te-I chemical potential space. (b,c) Defect diagrams (with formation energies of all intrinsic defects) calculated at chemical potentials corresponding to (b) PbTe-PbI_2-Pb and (c) PbTe-PbI_2-Te equilibria. The equilibrium Fermi levels ($E_{F,eq}$) at 973 K are included in both defect diagrams. The gray region represents the conduction band, and the calculated band gap (E_g) and conduction band minimum (CBM) are labelled in (b). Iodine interstitials are not shown in the plot, because they have very high formation energies (~ 5 eV) in the shown chemical potential space.