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Supporting Information

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Novel Polytype of III–VI Metal Chalcogenides Nano Crystals Realized in Epitaxially Grown InTe

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Supporting Information

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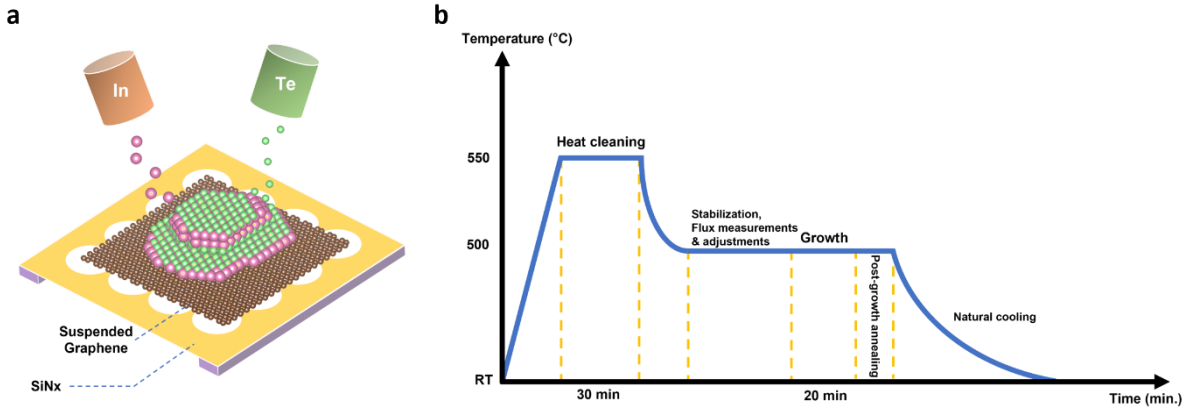

Figure S1 (a) Schematic of MBE process for InTe growth. The graphene/SiN membrane template was adopted as both substrate and TEM grid. Evaporated beams of In and Te atoms were deposited directly onto graphene. (b) MBE growth profile for InTe on graphene. The growth of InTe was performed as a single-step process after heat cleaning, followed by annealing and cooling.

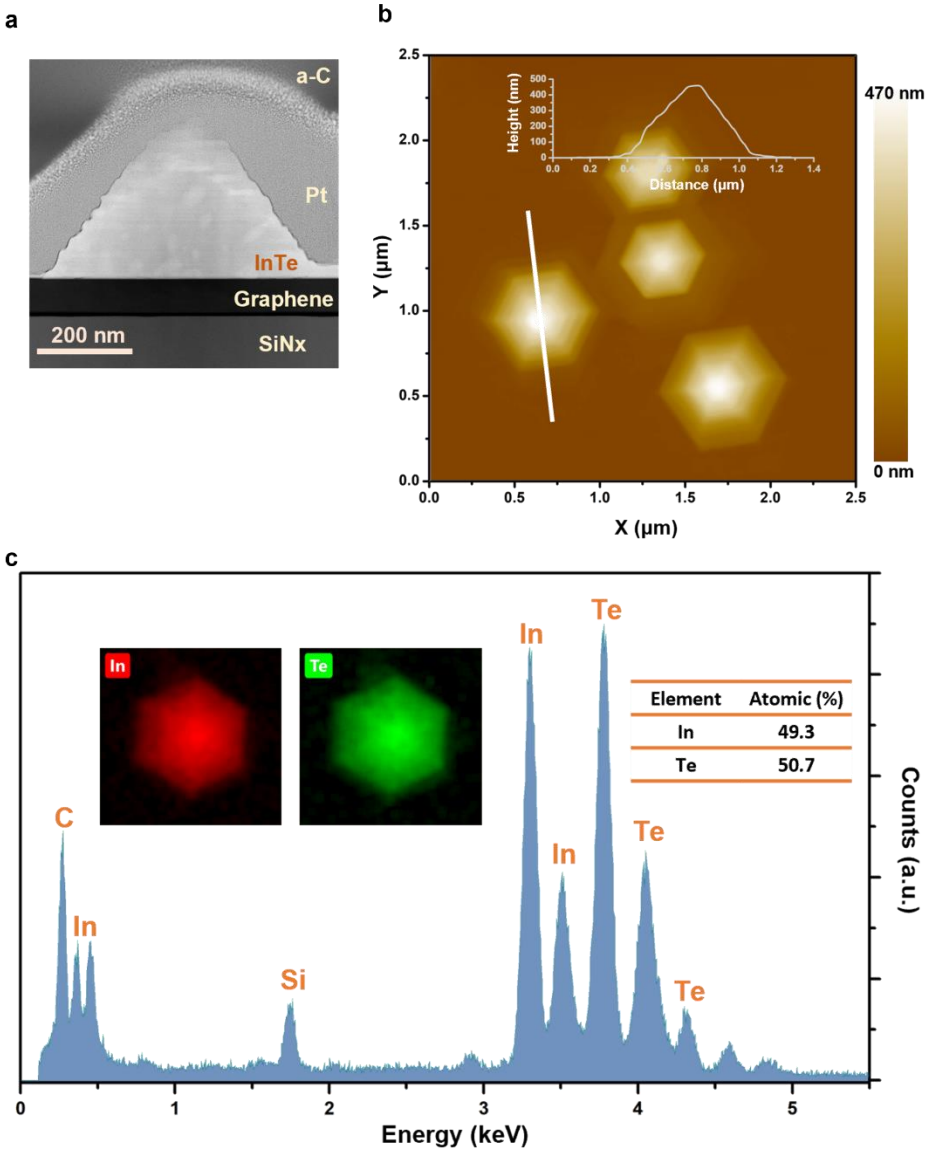

Figure S2 (a) STEM image of a cross-section of an InTe flake. InTe grew in a pyramid shape. (b) AFM image of InTe flakes. The inset presents a line profile along the white line in the image. (c) EDX spectrum obtained from an InTe flake. The atomic percentage shows that the stoichiometry of In and Te is 1:1. The inset images are the EDS mapping. Red and green represents In and Te atoms, respectively.

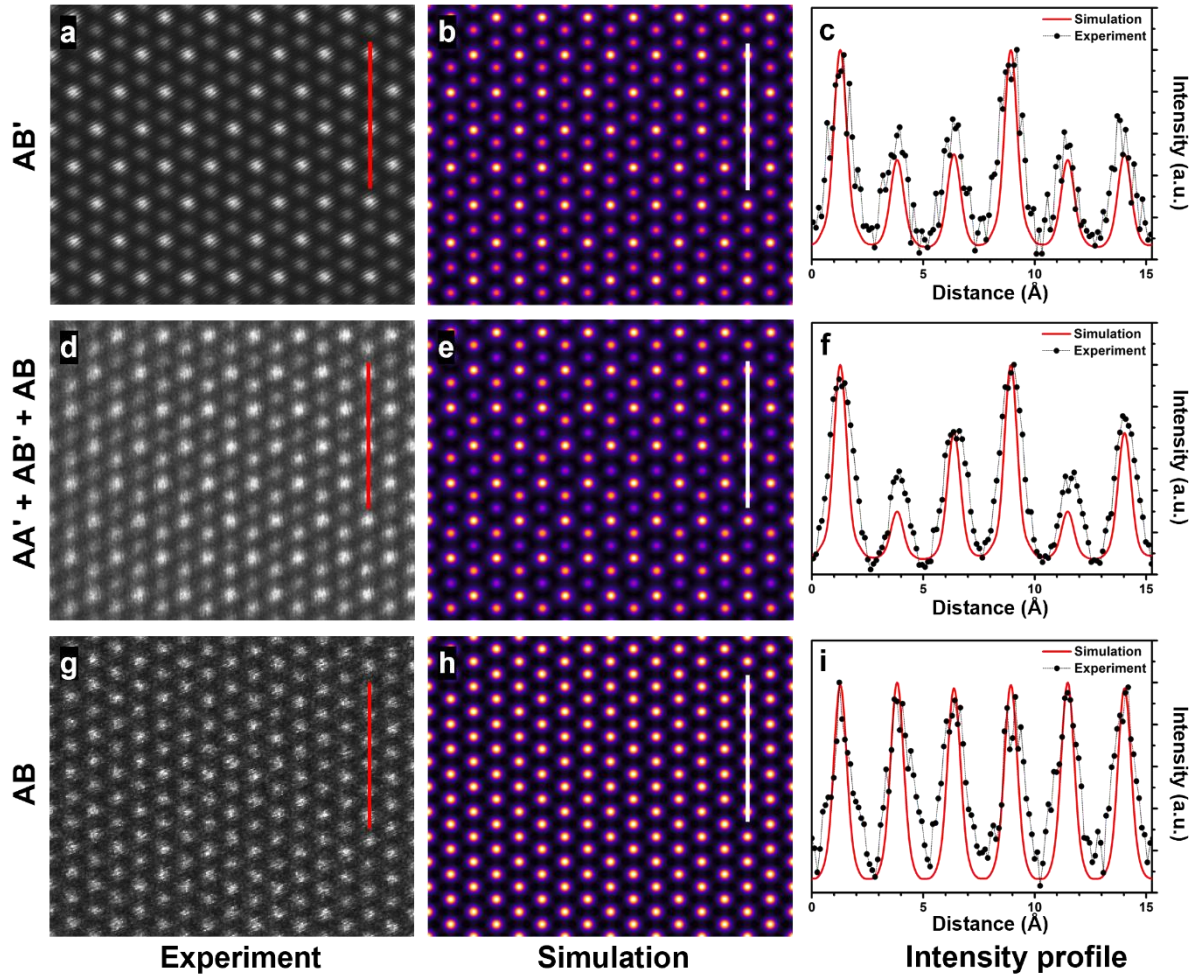

Figure S3 Atomic resolution structures of InTe crystals with different stacking modes. (a, d, g) STEM images obtained from regions with (a) AB′, (d) AA′ + AB + AB, and (g) AB stacking. (b, e, h) Simulated STEM images of (b) AB′, (e) AA′ + AB + AB, and (h) AB stacking. (c, f, i) Intensity profiles along the red solid line in the STEM images in a, d, g (scattered dots) and the white solid line in the simulated STEM images in b, e, g (solid curve). The two intensity profiles from the experiment and simulation agree well, suggesting the grown InTe exhibits a mixture of multiple stackings.

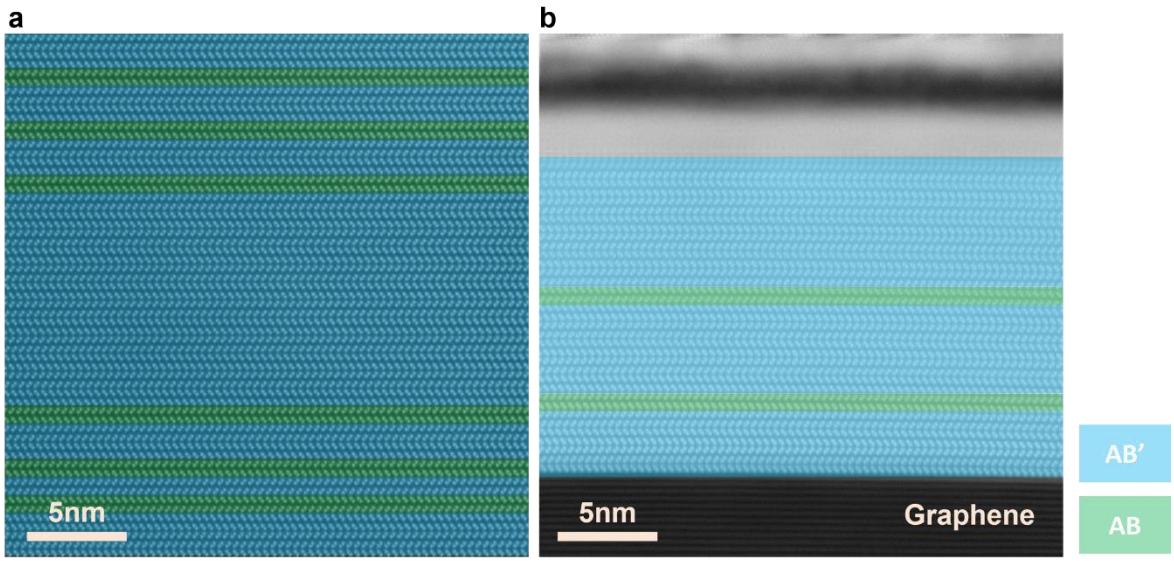

Figure S4 Distribution of AB′ and AB stacking in the middle of InTe flake (a) and near the graphene substrate (b). Blue and green regions represent AB′ and AB stackings, respectively. Regardless of the stage of growth, AB′ stacking is highly distributed.

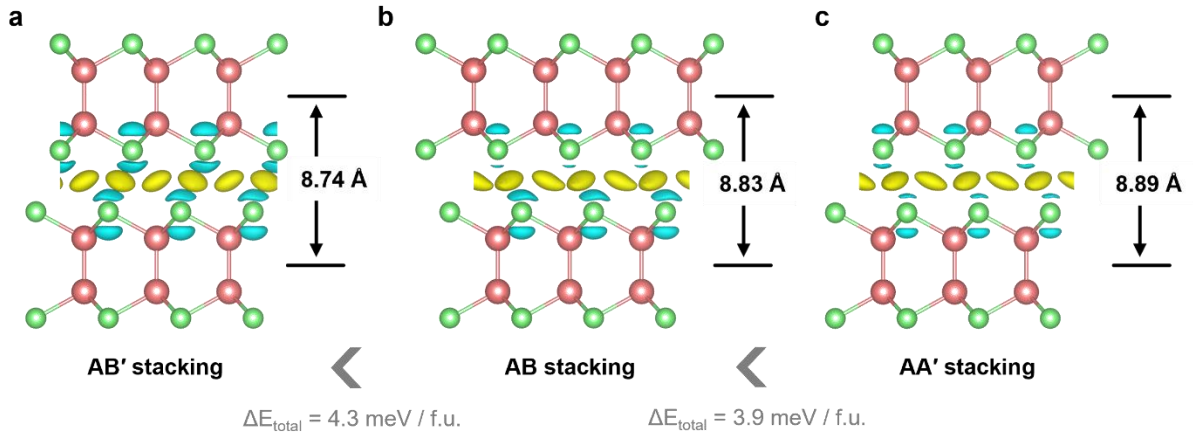

Figure S5 DFT results of interlayer distances, differential charge densities, and total energies of bilayer AA′, AB, and AB′ stacking, respectively. The isosurface value is set to 1.8×10^{-4} electrons per $Å^3$. The charge accumulation and depletion are shown in yellow and blue, respectively. AB′ stacking is 4.3 meV per formula unit (meV/f.u.) lower in total energy than AB stacking and is the most energetically stable, while AA′ stacking is 3.9 meV/f.u. higher than AB stacking and has the highest energy among the three stackings.

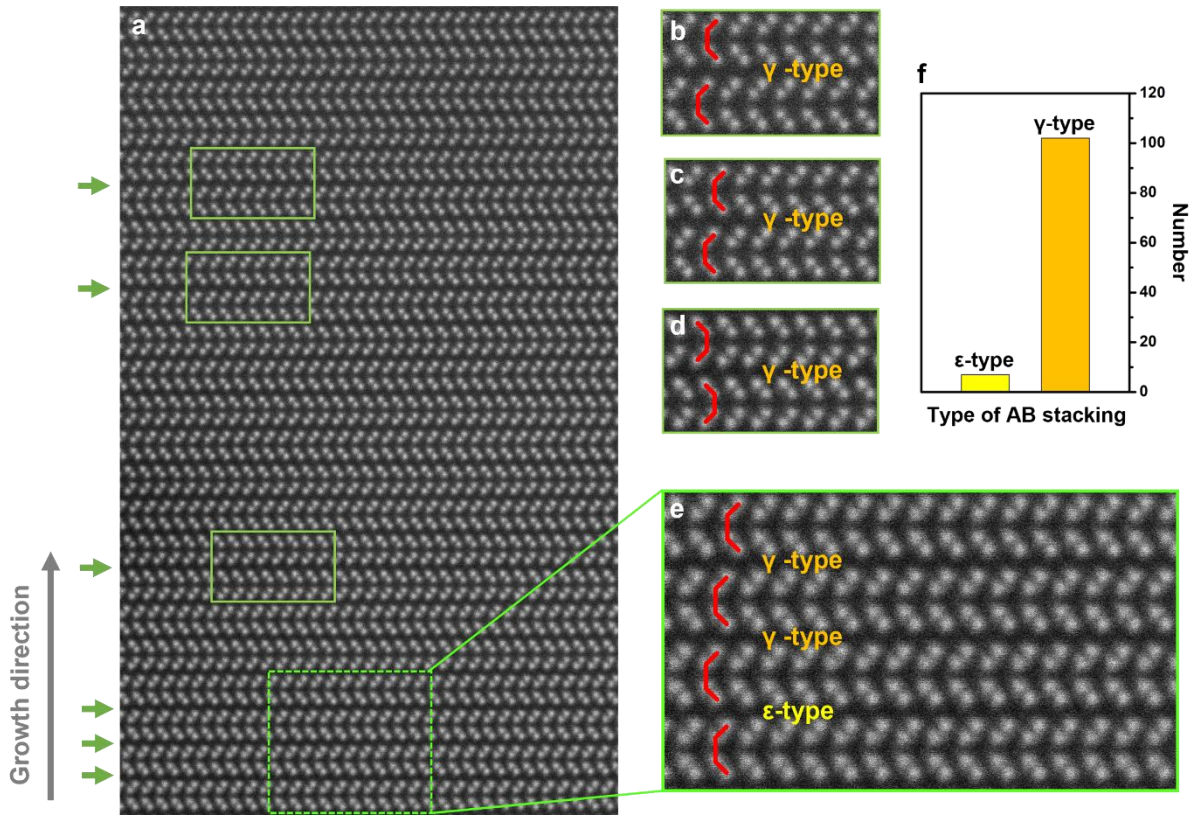

Figure S6 Two types of AB stacking with respect to growth direction (a) HAADF-STEM image of a region containing two types of AB stacking: ε-type and γ-type. Green arrows indicate AB stackings, and the other interlayers consist of AB′ stackings. The growth direction is denoted by the gray arrow. (b–e) Magnified images that show AB stackings corresponding to boxed regions in a. Red solid lines represent monolayer units. Depending on the growth direction, two types of AB stacking are clearly distinguished. Boxes with a dark green solid line indicate γ-type, and the box with the light green dashed line box indicates the region where ε-type is present. (f) Statistics of classified AB stackings showing that most AB stacking exhibits type γ.

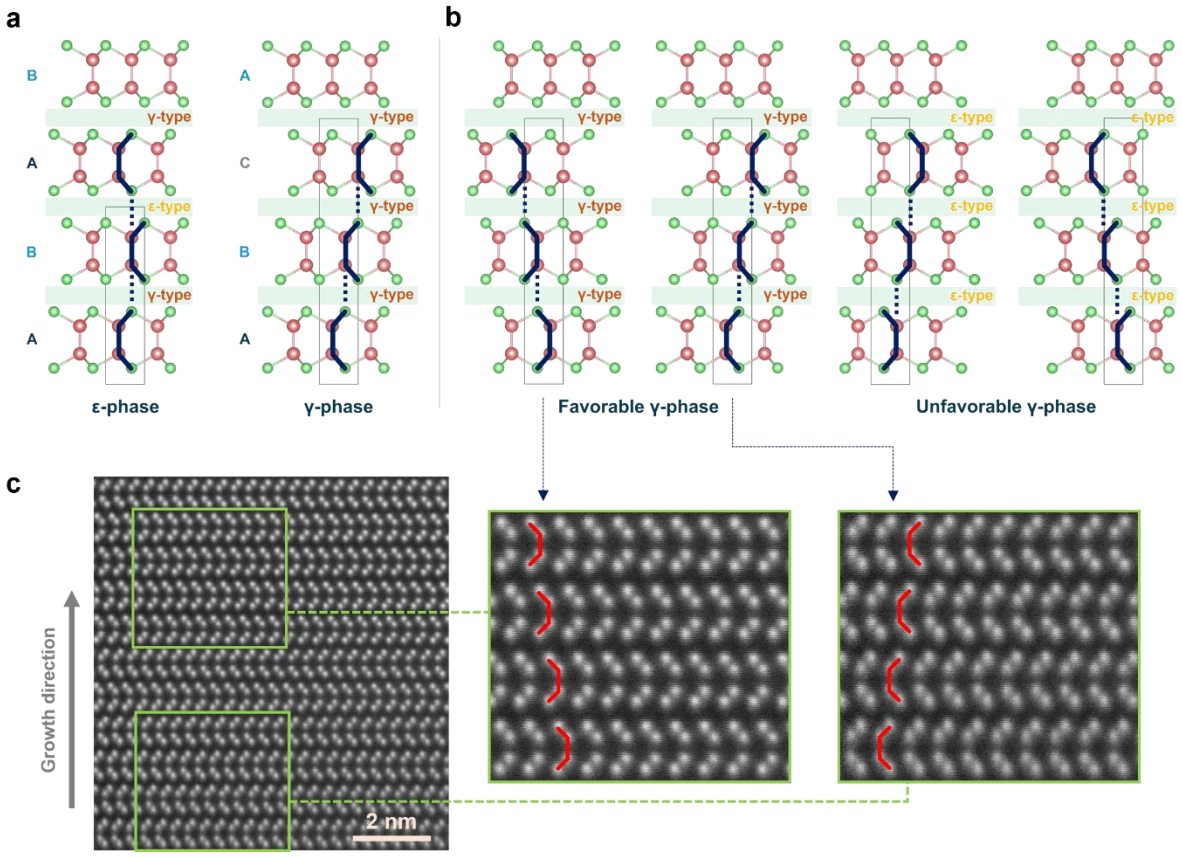

Figure S7 (a) ε-phase and γ-phase in terms of two types of AB stacking. ε-type AB stacking is indispensable for the ε-phase. Unlike the ε-phase, the γ-phase can be composed of only γ-type stacking. (b) Four different patterns of γ-phase regarding the direction of growth. Inequivalent types of AB stacking speak not only about the dominance of the γ-phase over the ε-phase but also about the preferred growth direction of the γ-phase. (c) HAADF-STEM image which exhibits two favorable γ-phase arrangements.