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Supplementary Materials

Tailoring the Structural and Optical Properties of Germanium Telluride Phase-Change Materials by Indium Incorporation

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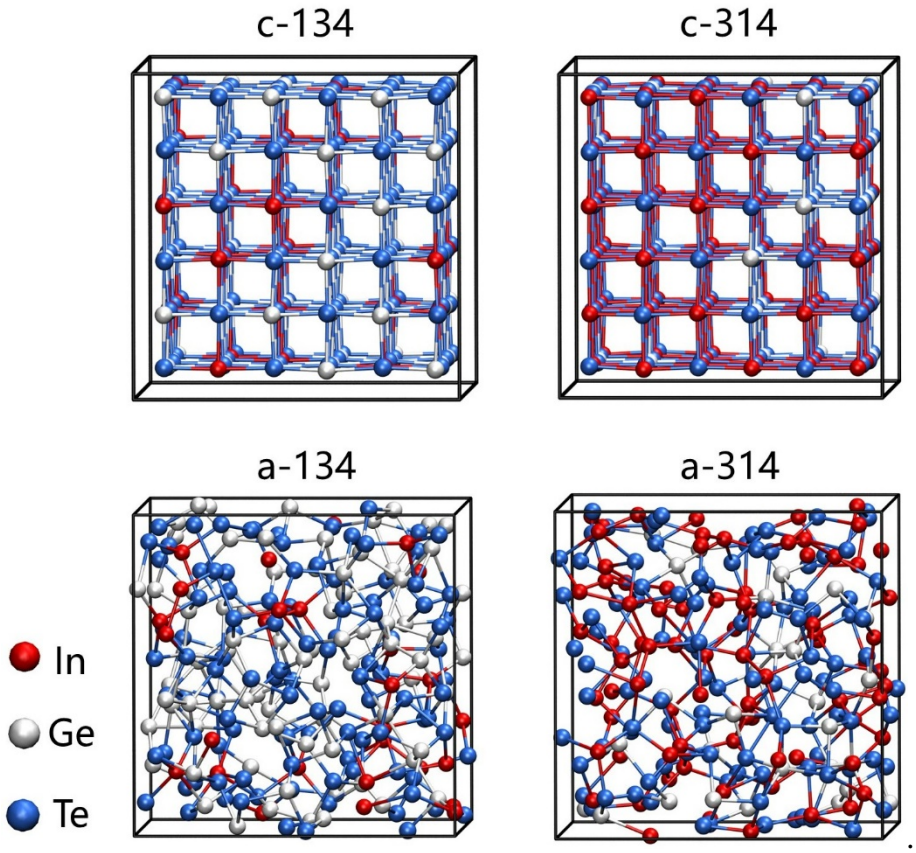

Figure S1. Atomic structures of crystalline and amorphous $InGe_3Te_4$ and In_3GeTe_4 (denoted as c/a-134 and 314).

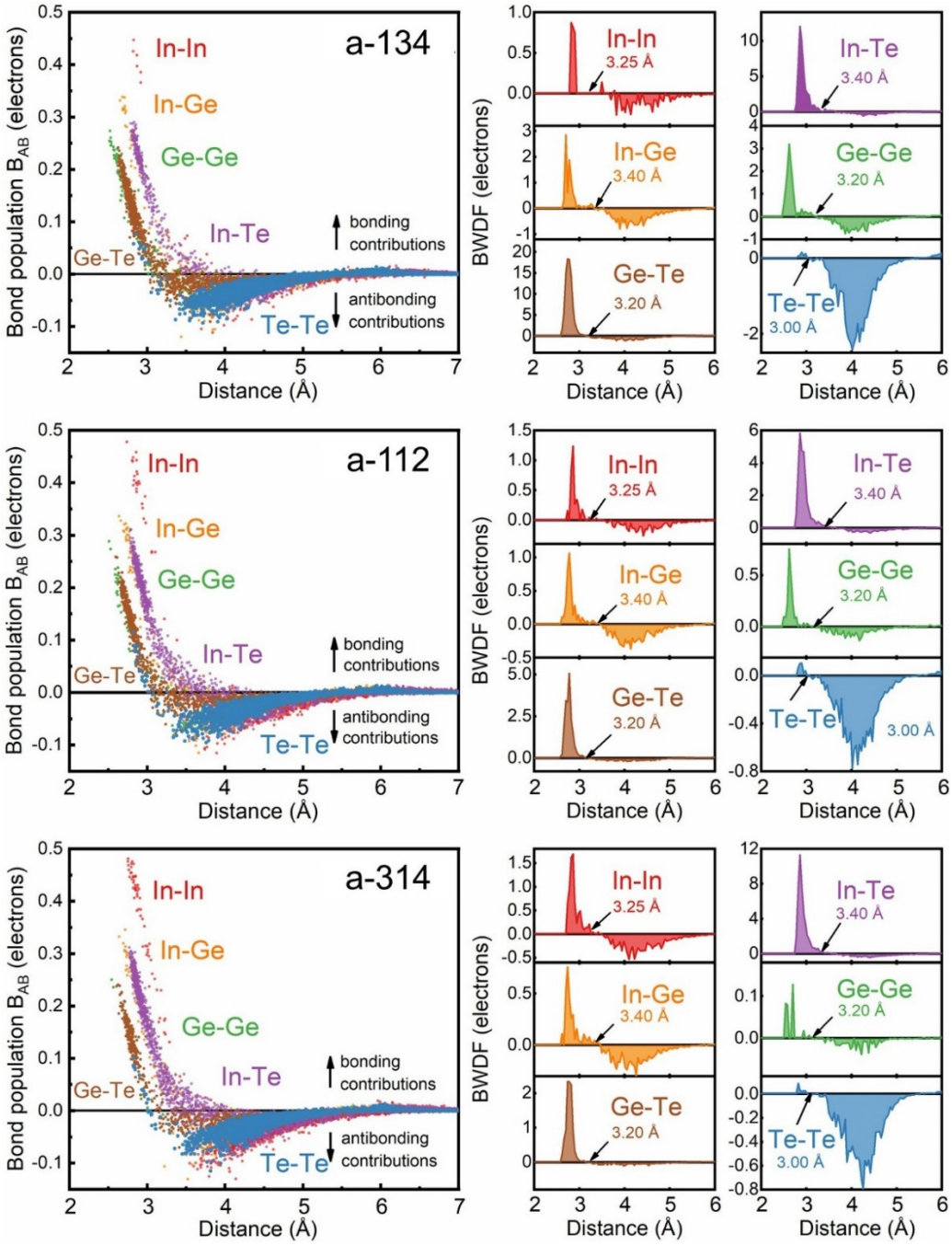

Figure S2. Bond population (left panel) and bond weighted distribution functions BWDFs (right panel) for each interatomic pair in the three amorphous compounds. The crossover values from positive to negative in the BWDFs represent cutoff values for bonding interactions, which are used for structural analysis. Further technical details about BWDF can be found in Ref. 79 of the main text.

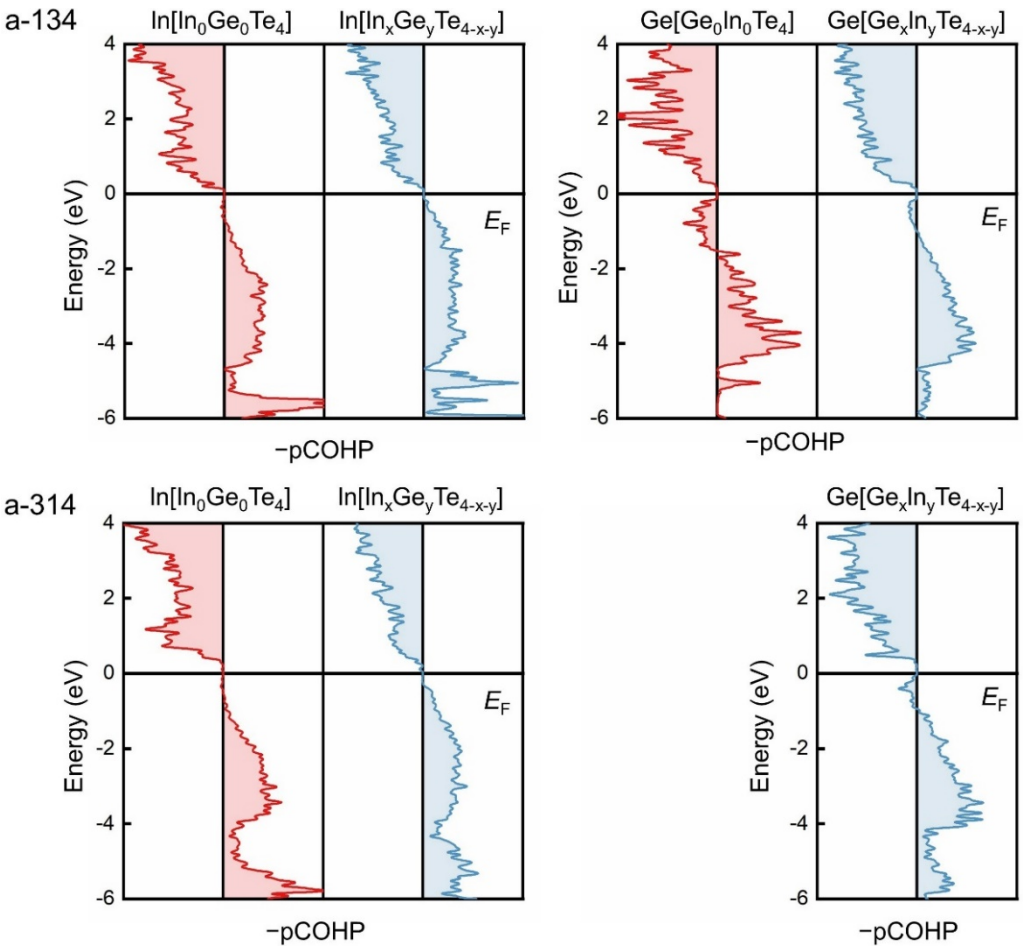

Figure S3. Projected COHP (pCOHP) for tetra-In and tetra-Ge motifs in a-$InGe_3Te_4$ and a-In_3GeTe_4. Tetrahedral motifs are grouped as the ones with only heteropolar bonds, denoted as $In[In_0Ge_0Te_4]$ and $Ge[Ge_0In_0Te_4]$, and the others with at least one wrong bond indicated as $In[In_xGe_yTe_{4-x-y}]$ and $Ge[Ge_xIn_yTe_{4-x-y}]$ (x or y ≥1, x+y≤4). In the a-314 structure, $Ge[Ge_0In_0Te_4]$ motif is absent.

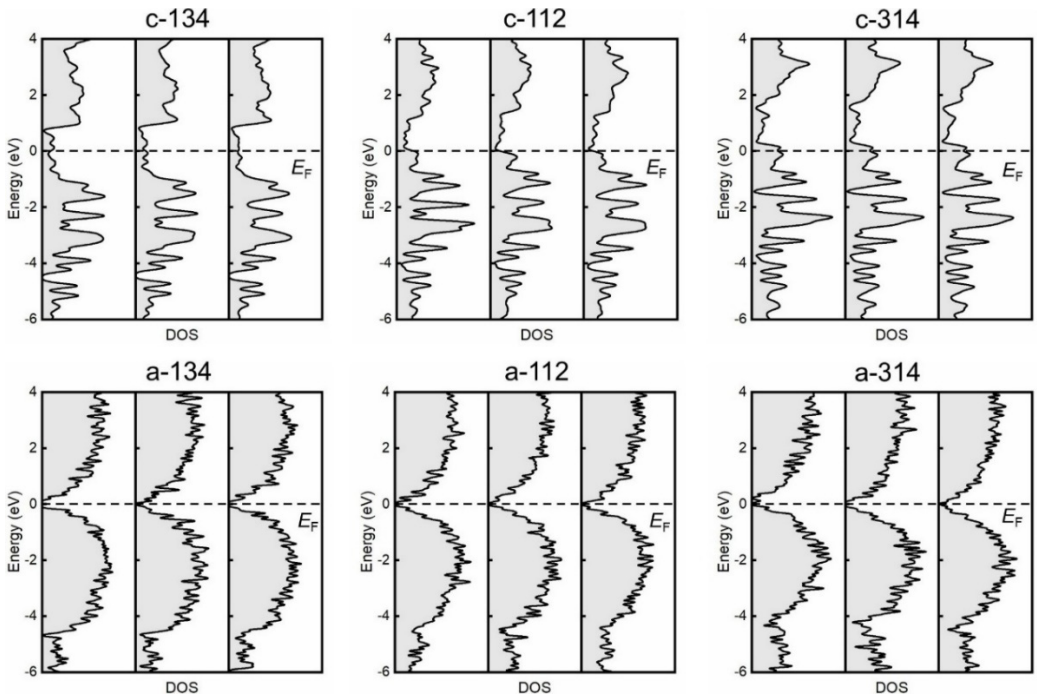

Figure S4. Density of states (DOS) for crystalline and amorphous structures of the three IGT compositions. Three models for each composition were built, which show consistent results.