Supplementary Information

For

Competing ionic and covalent bonding in Ge-Sb-Te phase change materials

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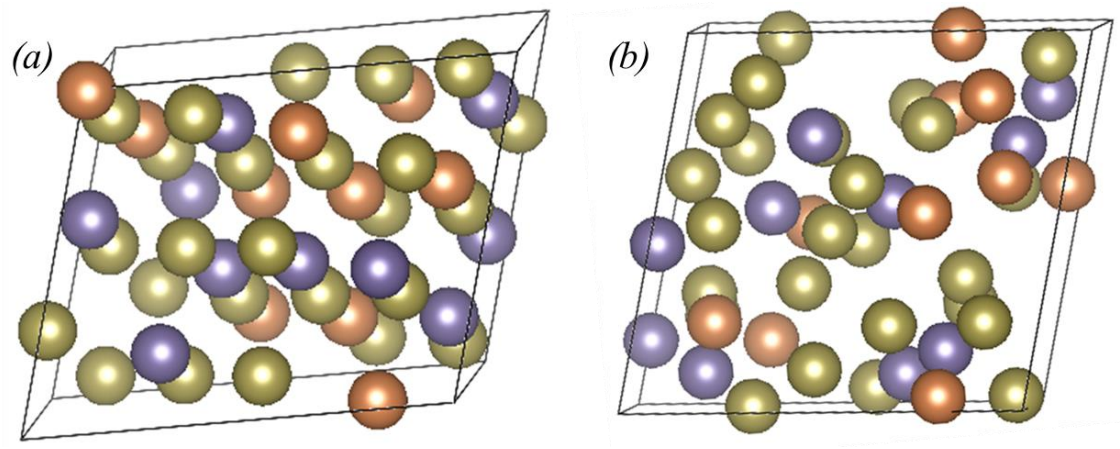

Figure S1: Optimized configuration of (a) c-GST and (b) a-GST. The violet, orange and brown spheres represent the Ge, Sb and Te atoms.

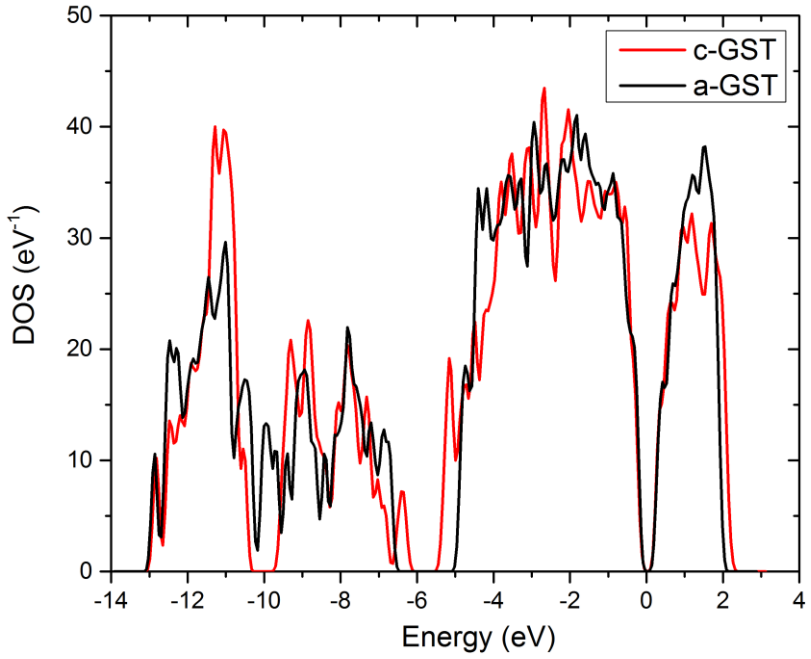

Figure S2: Total density of states of c-GST (red line) and a-GST (black line) calculated with PBE-GGA.

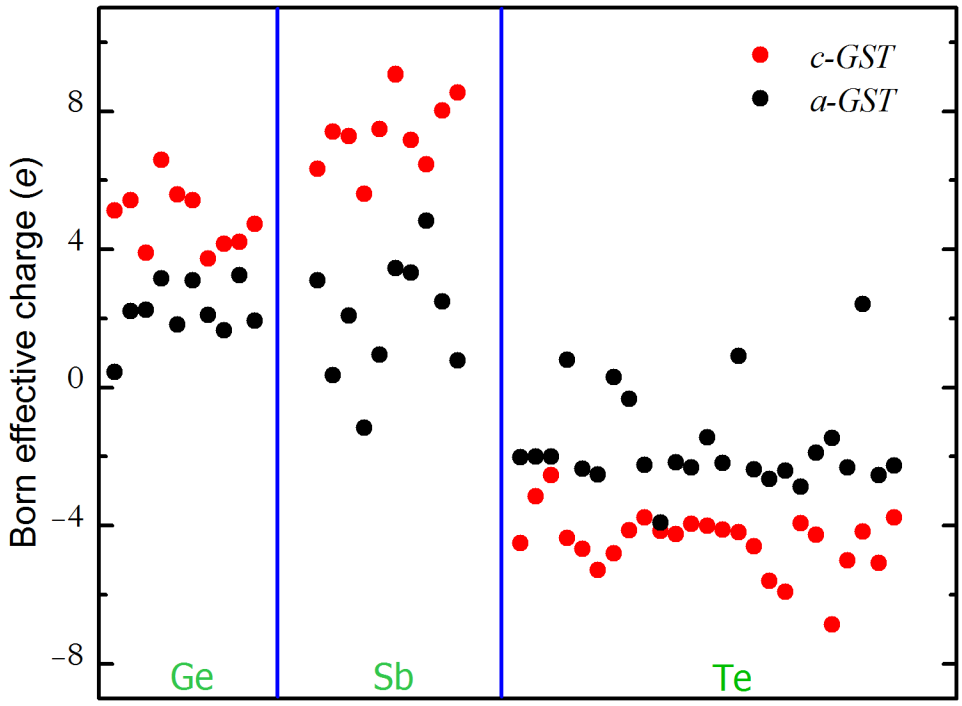

Figure S3: Born effective charges on Ge, Sb and Te atoms in c-GST and a-GST. Red and black spheres stand for Born effective charges in c-GST and a-GST, respectively.

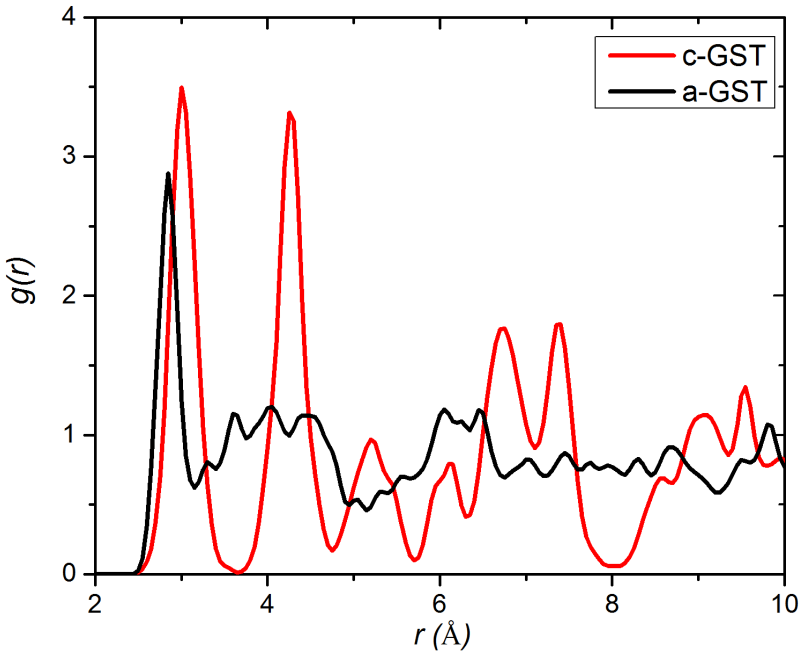

Figure S4: Pair correlation functions for c-GST and a-GST.