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Supplementary Information

For

## Chemical understanding of resistance drift suppression in Ge-

## **Sn-Te phase-change memory materials**

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**Figure S1.** The ground state calculations of crystalline GeTe and SnTe at 0 K. Both crystals are in a rhombohedral structure, where the distortion is much stronger in GeTe than in SnTe. For GeTe, the lattice parameter is 4.37 Å, the lattice angle is 57.9°, the relative positions of Ge and Te are (0,0,0) and (0.53, 0.53, 0.53), the bond lengths are 2.86 and 3.25 Å, and the Mulliken charges (in electrons per atom) of Ge and Te are +0.03 and -0.03. For SnTe, the lattice parameter is 4.54 Å, the lattice angle is 59.8°, the relative positions of Sn and Te are (0, 0, 0) and (0.51, 0.51, 0.51), the bond lengths are 3.14 and 3.27 Å, and the Mulliken charges of Sn and Te are +0.27 and -0.27.



**Figure S2.** The Mulliken Charge (in electrons per atom) profile of 3-fold defective octahedral Te atoms with different neighboring configuration in amorphous GeSnTe<sub>2</sub>: the more Sn neighbors, the larger the charge transfer.



**Figure S3.** The projected crystal orbital overlap population over different tetrahedral motifs in amorphous SnTe. A high antibonding is found in the tetrahedral Sn[Te<sub>4</sub>Sn<sub>0</sub>] motifs, which is reduced largely with presence of homopolar bonds in tetrahedral Sn[Te<sub>3</sub>Sn<sub>1</sub>] motifs. In fact, the tetrahedral Sn[Te<sub>4</sub>Sn<sub>0</sub>] motif is rarely found in the whole amorphous network.



**Figure S4.** The detailed analyses of 4-fold primitive rings in amorphous GeTe, GeSnTe<sub>2</sub> and SnTe. The fraction of ABAB rings (A = Ge or Sn, B = Te) increases gradually upon Sn substitutions. Non-ABAB rings are mostly made of AAAB and ABBB rings.