

Supporting Information for

High-throughput screening to identify two-dimensional layered phase-change chalcogenides for embedded memory applications

Suyang Sun^{1#}, Xiaozhe Wang^{1#}, Yihui Jiang^{1,2}, Yibo Lei², Siyu Zhang¹, Sanjay Kumar¹, Junying Zhang¹, En Ma¹, Riccardo Mazzarello³, Jiang-Jing Wang^{1,*}, Wei Zhang^{1,*}

¹Center for Alloy Innovation and Design (CAID), State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, China.

²Key Laboratory of Synthetic and Natural Functional Molecule of the Ministry of Education, College of Chemistry & Materials Science, Shaanxi key Laboratory of Physico-Inorganic Chemistry, Northwest University, Xi'an 710127, Shaanxi, P. R. China

³Department of Physics, Sapienza University of Rome, Rome 00185, Italy

*Emails: j.wang@mail.xjtu.edu.cn, wzhang0@mail.xjtu.edu.cn

#These authors contributed equally to this work.

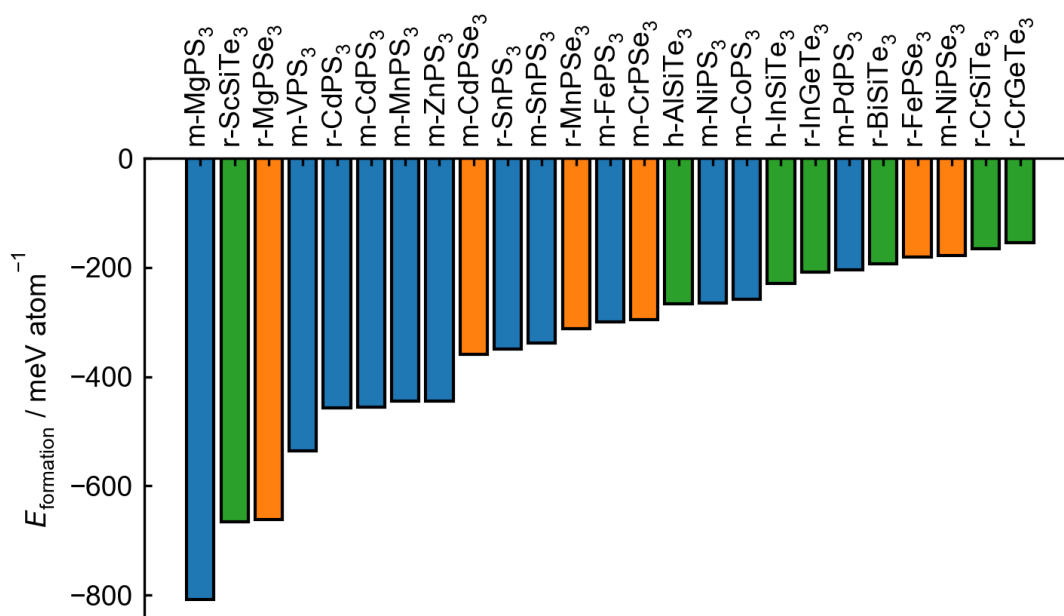


Figure S1. The formation energy of ABCh₃ referring to the ground-state elements, with sulfides, selenides, and tellurides being plotted in blue, orange and green respectively.

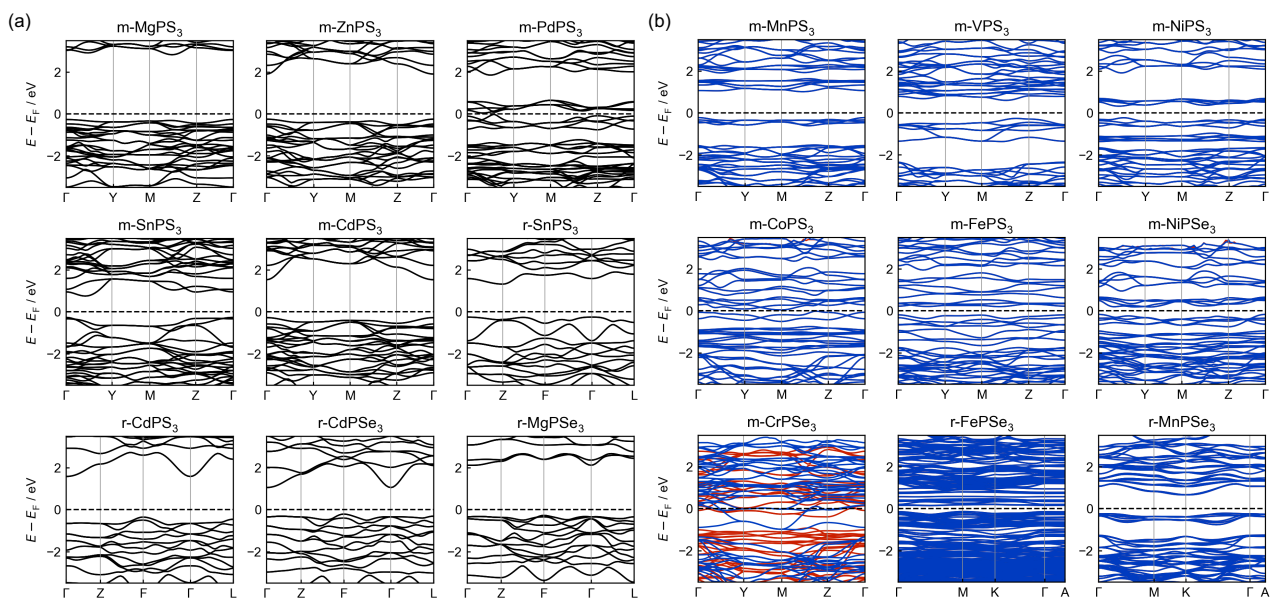


Figure S2. Calculated band structures of layered sulfides and selenides listed in Table 1. The non-magnetic and magnetic compounds are plotted in (a) and (b), respectively. Intralayer AFM configurations were considered.

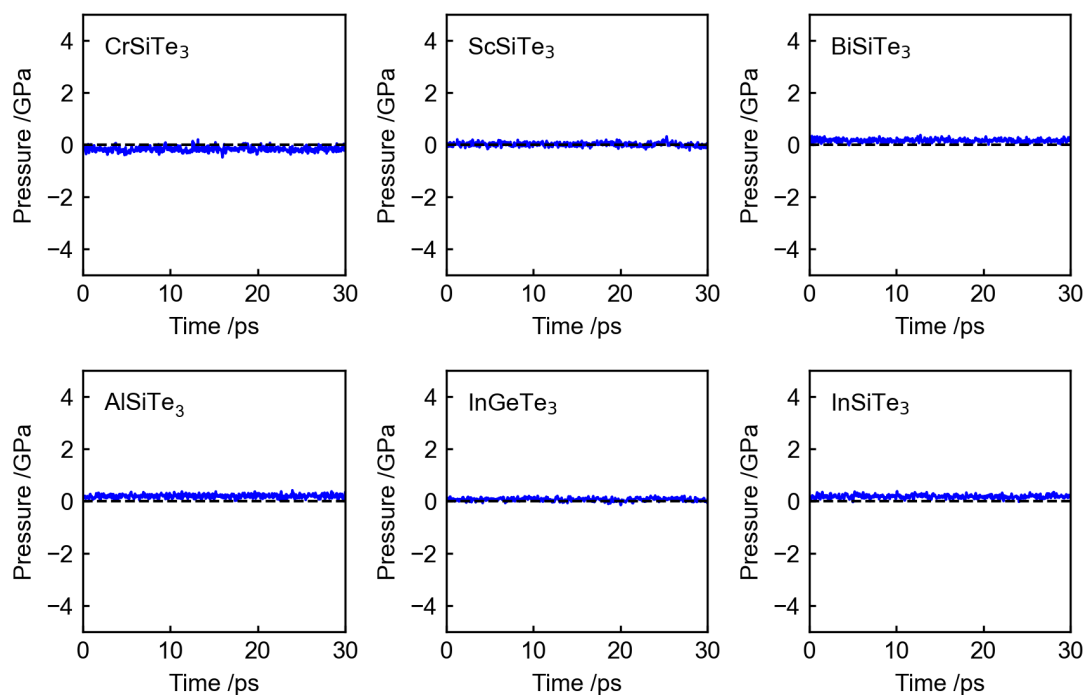


Figure S3. The internal pressure of the six amorphous tellurides models during annealing at 300K.

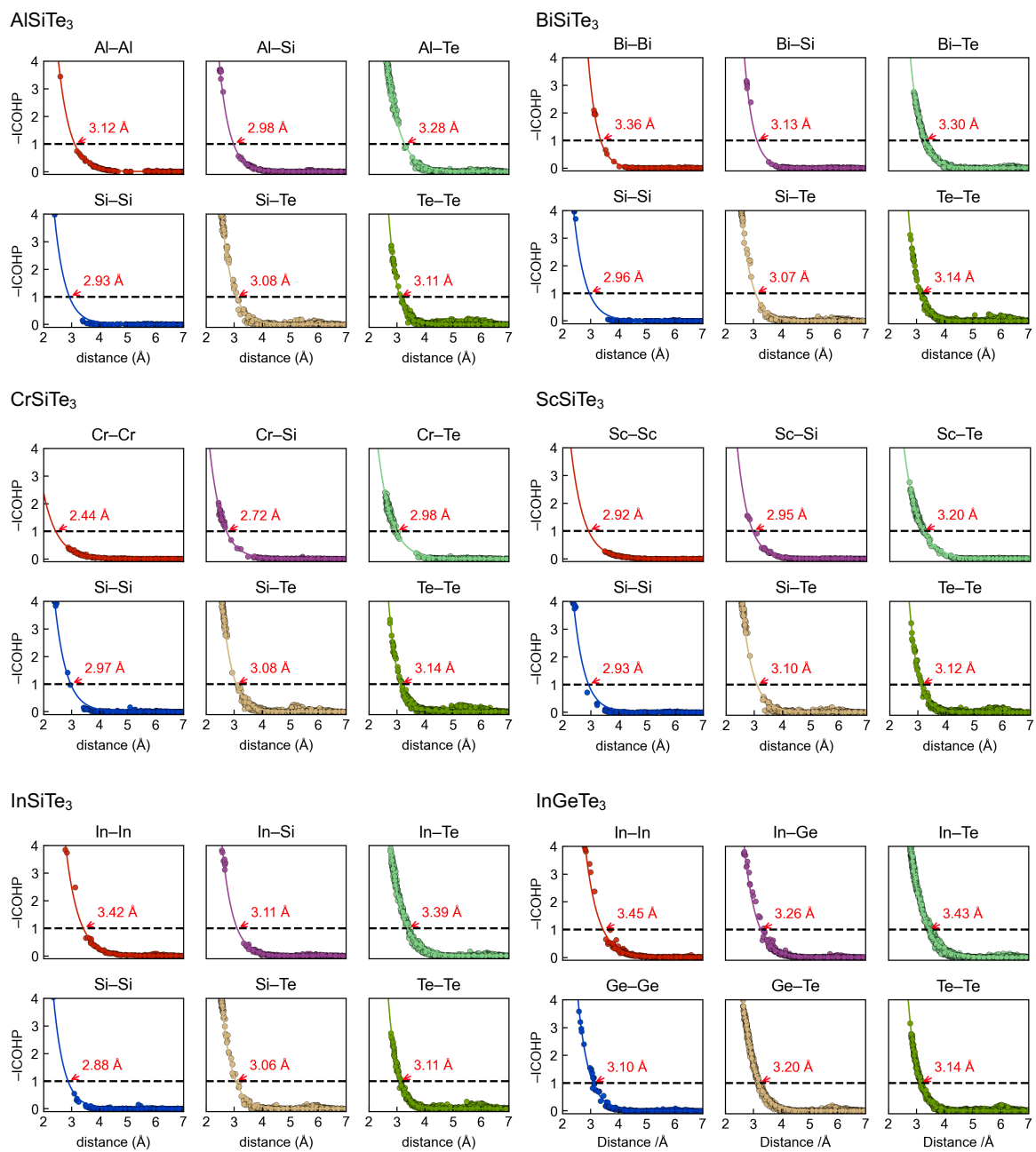


Figure S4. Element-specific cutoffs for interatomic distance determined using the $-\text{COHP}$ integral method.

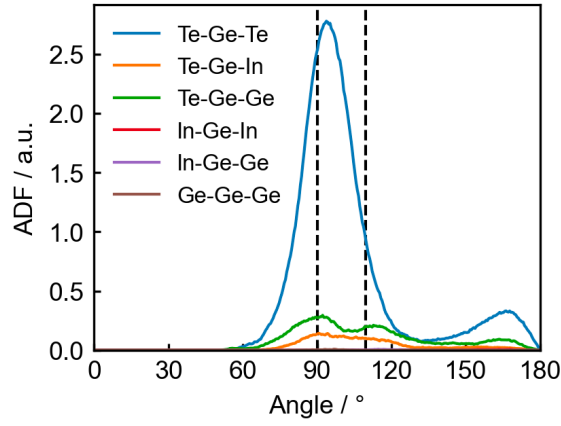


Figure S5. The element-specific ADF profiles around Ge atoms in amorphous InGeTe₃ models.

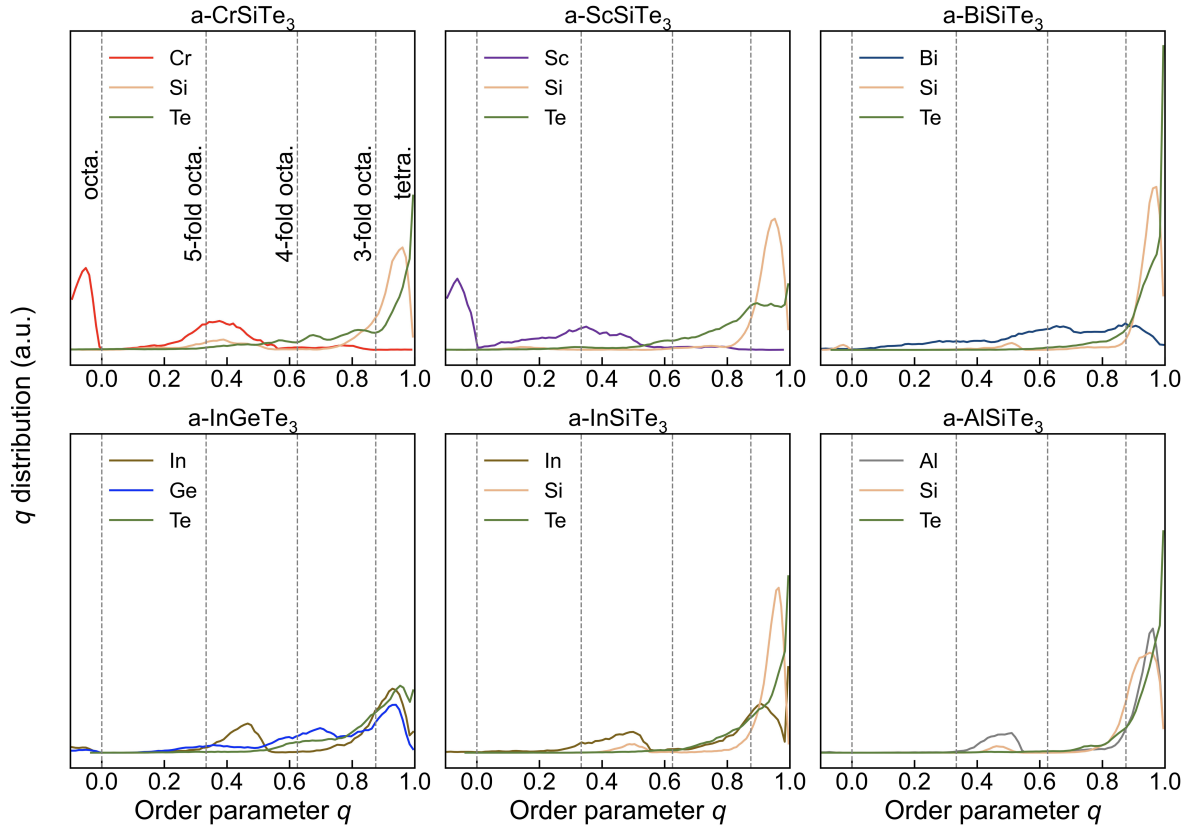


Figure S6. Element-specific bond-order parameters q calculated for the six amorphous alloys. The motifs of 6-, 5-, 4- and 3-fold (defective) octahedral (octa.) configurations corresponds to q value around 0, $1/3$, $5/8$ and $7/8$. Typical tetrahedral (tetra.) configurations have q values around 1.