# Supplement materials:

# Polyamorphism in $K_2Sb_8Se_{13}$ for multi-level phase-change memory

Meng Xu,[1] Chong Qiao,[1] Kan-Hao Xue, [1] Hao Tong,[1] Xiaomin Cheng,[1] Songyou Wang,[2] Cai-Zhuang Wang,[3] Kai-Ming Ho,[3] Ming Xu,[1,*] and Xiangshui Miao[1]

[1]*Wuhan National Laboratory for optoelectronics, School of Optical and Electronic Information, Huazhong University of Science and Technology, Wuhan 430074, China*

[2]*Shanghai Ultra-Precision Optical Manufacturing Engineering Center and Department of Optical Science and Engineering, Fudan University, Shanghai, 200433, China*

[3]*Ames Laboratory, U. S. Department of Energy and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*

***Email: mxu@hust.edu.cn**

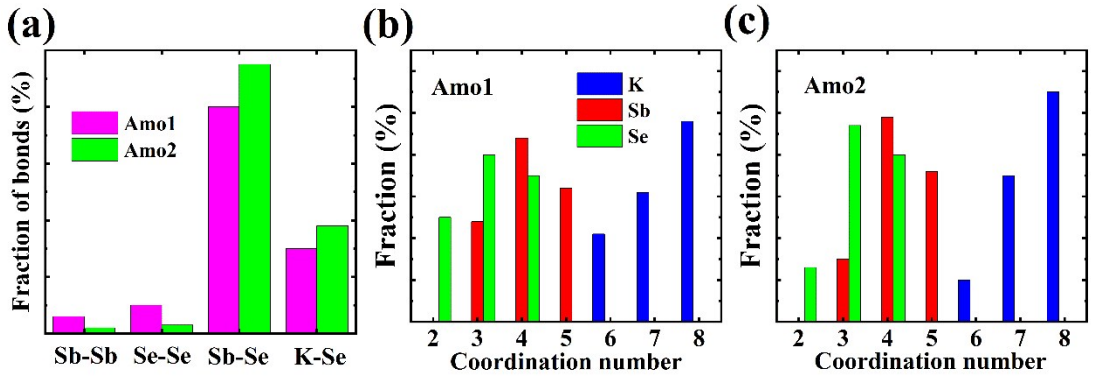


Figure S1 a) Distribution of various bonds in Amo1 and Amo2. It shows the decrease of Sb-Sb and Se-Se bonds and increase of Sb-Se and K-Se bonds in Amo2. b-c) Distribution of coordination number of two amorphous states, showing the increase of atoms that have more nearest neighbors in Amo2.

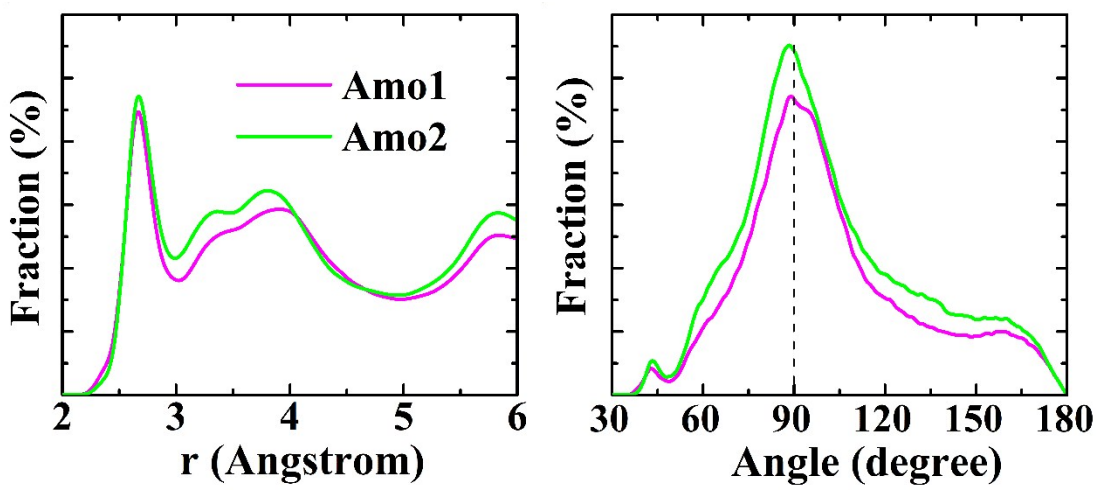


Figure S2. Average PDFs and ADFs of Amo1 and Amo2.

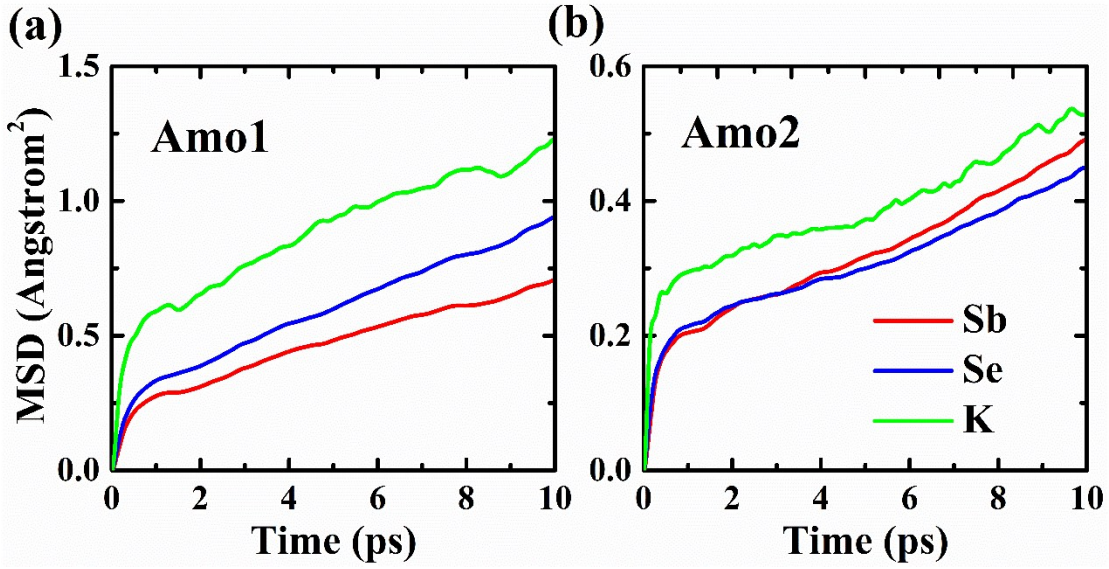


Figure S3. Mean square displacement (MSD) of Amo1 (a) and Amo2 (b). The diffusivity of atoms in Amo1 seems faster than that in Amo2.

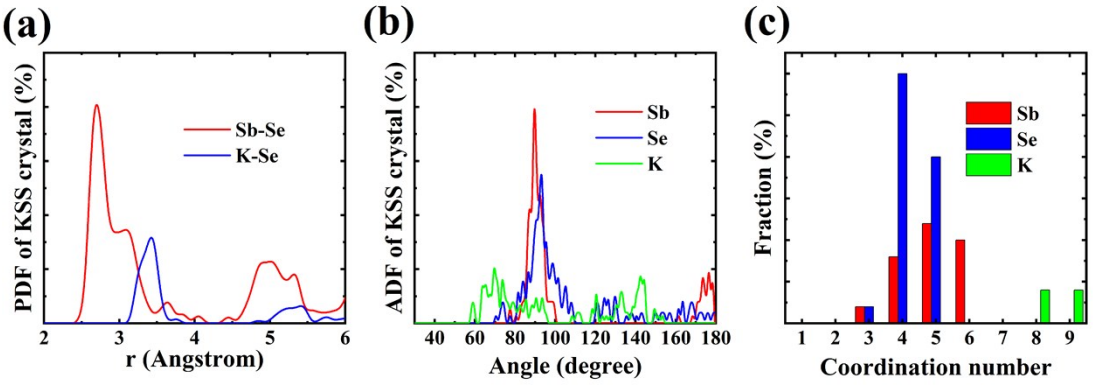


Figure S4. Pair distribution function, angle distribution function, and distribution of coordination number of KSS crystal. a) The K-Se bonds are longer than Sb-Se bonds. b) Sb and Se atoms mainly form 90$^o$ angles and K atoms form smaller bonds. c) All types of elements have greater CN than both two amorphous states. It confirms that the Amo2 structure is closer to crystal than Amo1.

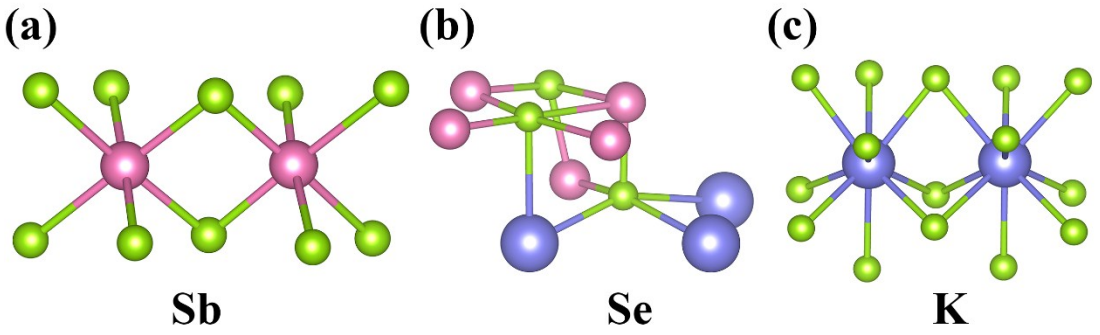


Figure S5. Local structure of Sb, Se, and K in KSS crystal. It shows Sb forms the octahedral motifs and the four-fold ring connects the octahedrons. Some Sb (CN < 6) form defective octahedral motifs. Se forms distorted octahedral motifs and four-fold rings. There exist 9 (or 8) Se atoms surround K uniformly and form distorted four-fold rings.

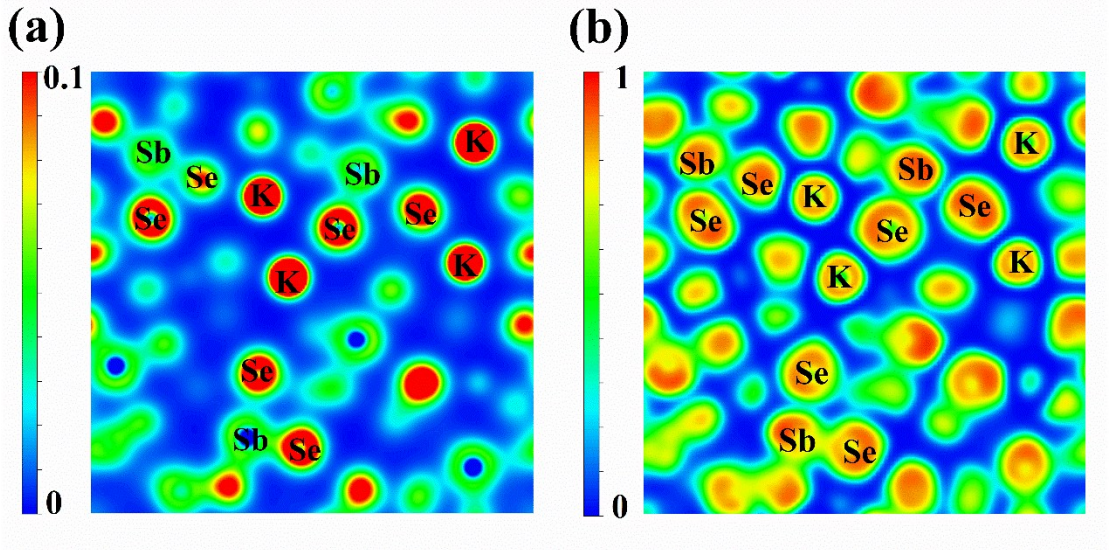


Figure S6. a) Charge density distribution of (100) plane of Amo2. b) ELF of (100) plane of Amo2.

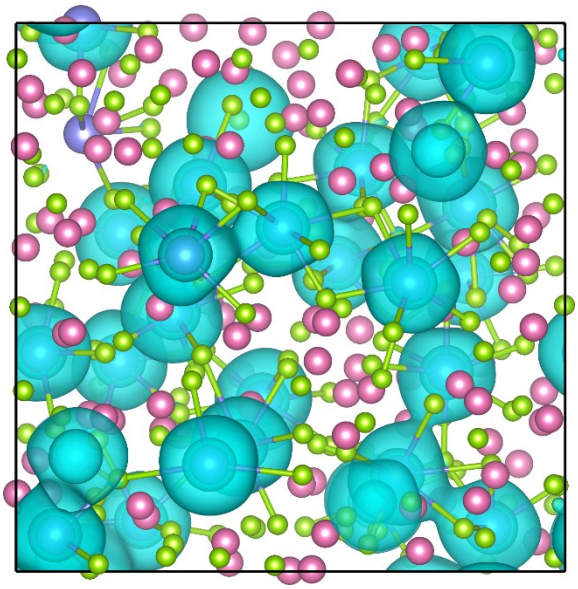

Figure S7. 3D display of charge density difference of Amo2.

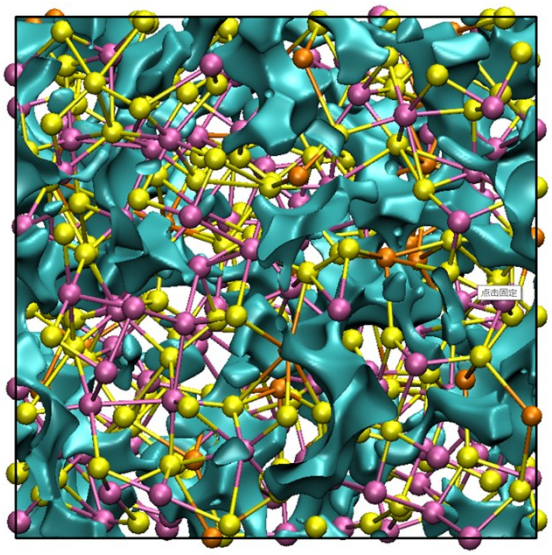

Figure S8. Void distribution of Amo2 by low electron density region.

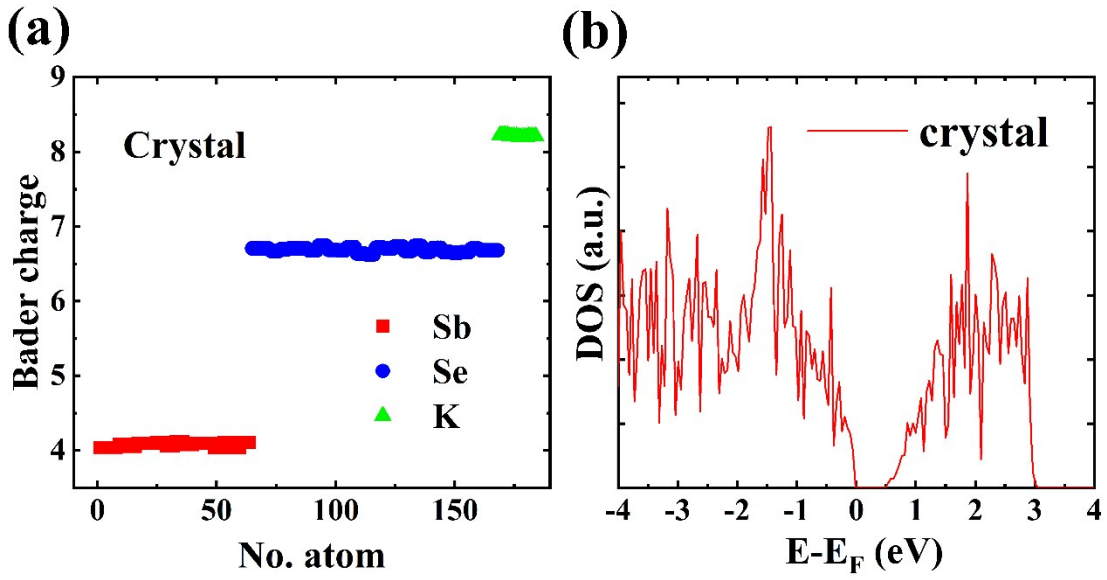


Figure S9. Bader change distribution and DOS of KSS crystal. Bader change distribution shows that Sb and K lose electrons while Se gets electrons. The bandgap of KSS crystal is about 0.5 eV, smaller than Amo2.

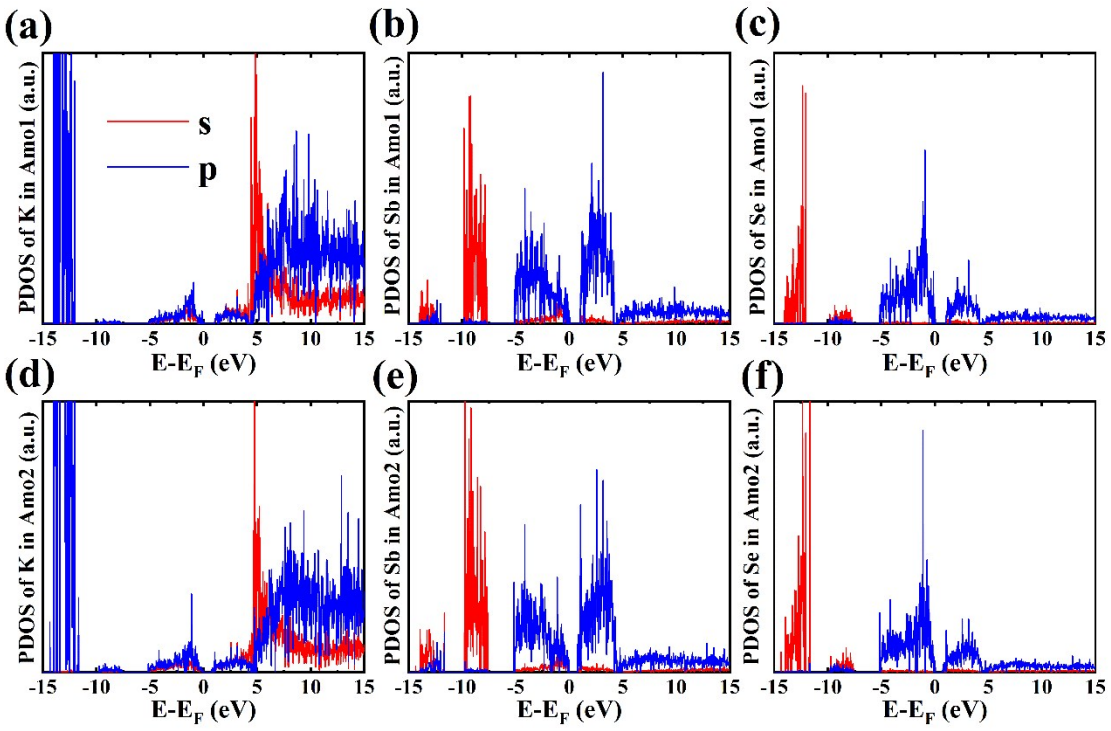


Figure S10. PDOS of various elements of both Amo1 and Amo2. It shows a little *s*-*p* hybrid orbitals in both states, and *p* orbitals play an important role in the bottom of conduction band, which leads to the decrease of bandgap in Amo2.

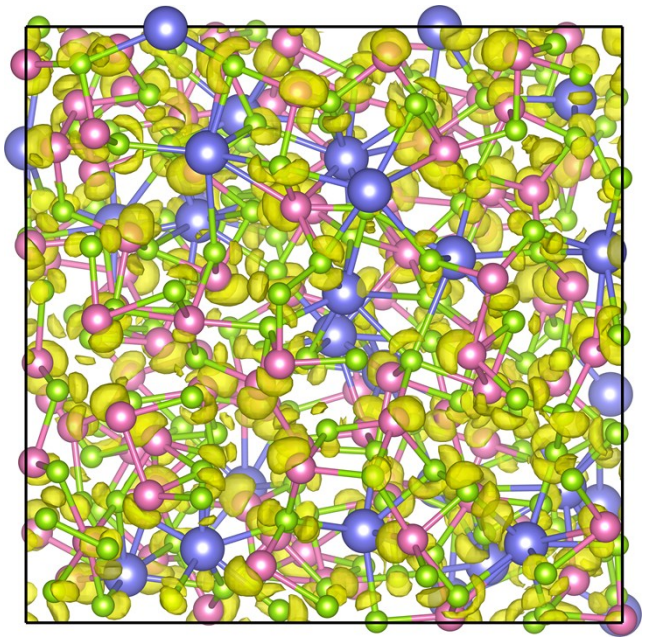

Figure S11. 3D display of electron localization function (isosurface = 0.85) of Amo2.

The yellow areas represent the lone pairs.