Supporting Information

High Thermoelectric Performance in Complex Phosphides Enabled by Stereochemically Active Lone Pair Electrons

Xingchen Shen,[a,f,†] Yi Xia, [b,†] Guiwen Wang,[c] Fei Zhou,[d] Vidvuds Ozolins,[e] Xu Lu, [a,*] Guoyu Wang,[f,*] Xiaoyuan Zhou, [a,c,*]

[a] Chongqing Key Laboratory of Soft Condensed Matter Physics and Smart Materials，College of Physics, Chongqing University, Chongqing, Chongqing 401331, P. R. China
[b] Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA
[c] Analytical and Testing Center of Chongqing University, Chongqing 401331, P. R. China
[d] Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, California 94550, USA
[e] Department of Applied Physics, Yale University, New Haven, Connecticut 06511, USA, and Energy Sciences Institute, Yale University, West Haven, Connecticut 06516, USA
[f] Chongqing Institute of Green and Intelligent Technology, Chinese Academy of Sciences Chongqing 400714, P. R. China and University of Chinese Academy of Sciences, Beijing, 100044, P. R. China

† X. S. and Y. X. contributed equally to this work.
* Corresponding author: luxu@cqu.edu.cn; guoyuw@cigit.ac.cn; xiaoyuan2013@cqu.edu.cn

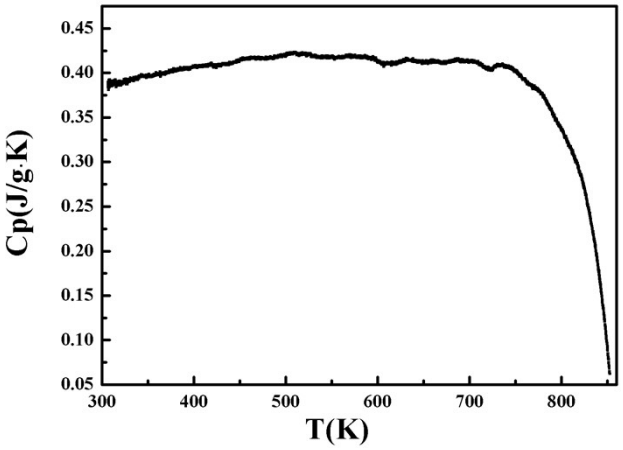

Fig. S1. Measured heat capacity of $Ag_6Ge_{10}P_{12}$.

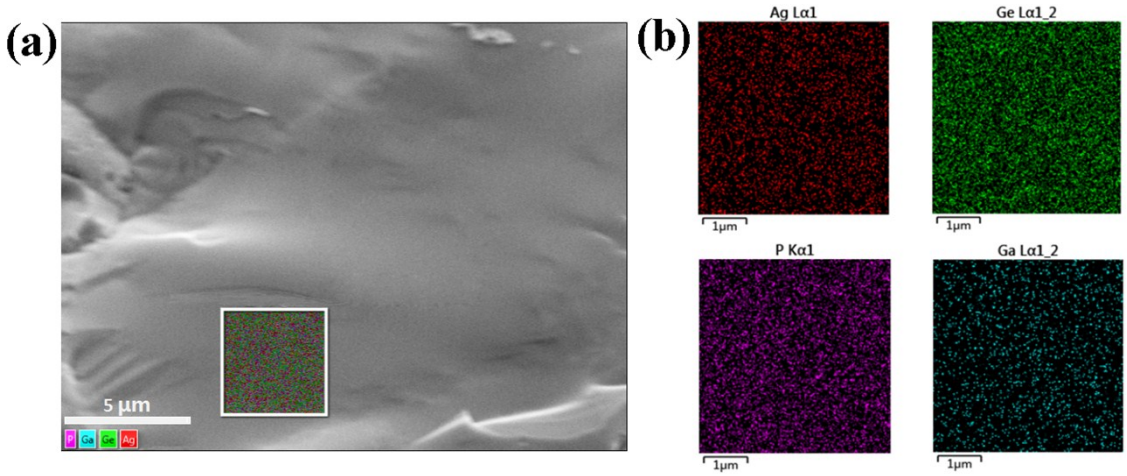

Fig. S2. (a, b) SEM-EDX elemental mapping images of the surface of $Ag_6Ge_{9.7}Ga_{0.3}P_{12}$.

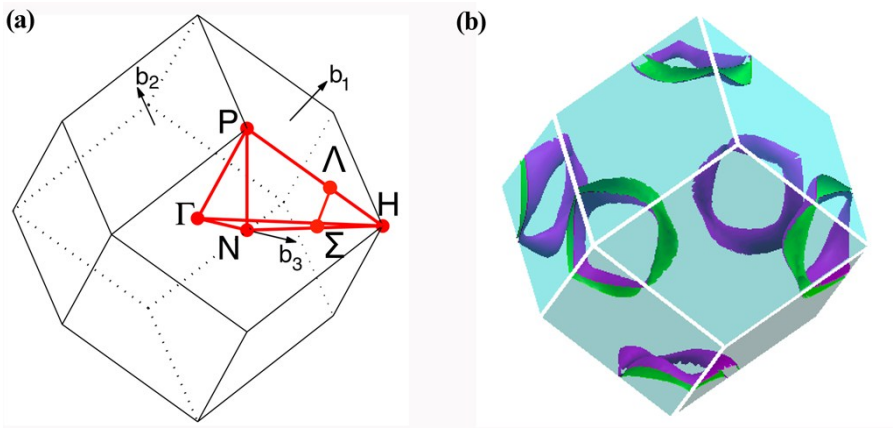

Fig. S3. (a) Brillouin zone of the bcc unit cell of $Ag_6Ge_{10}P_{12}$; (b) Fermi surface of hole carriers for the Fermi level set at 50 meV below the VBM.

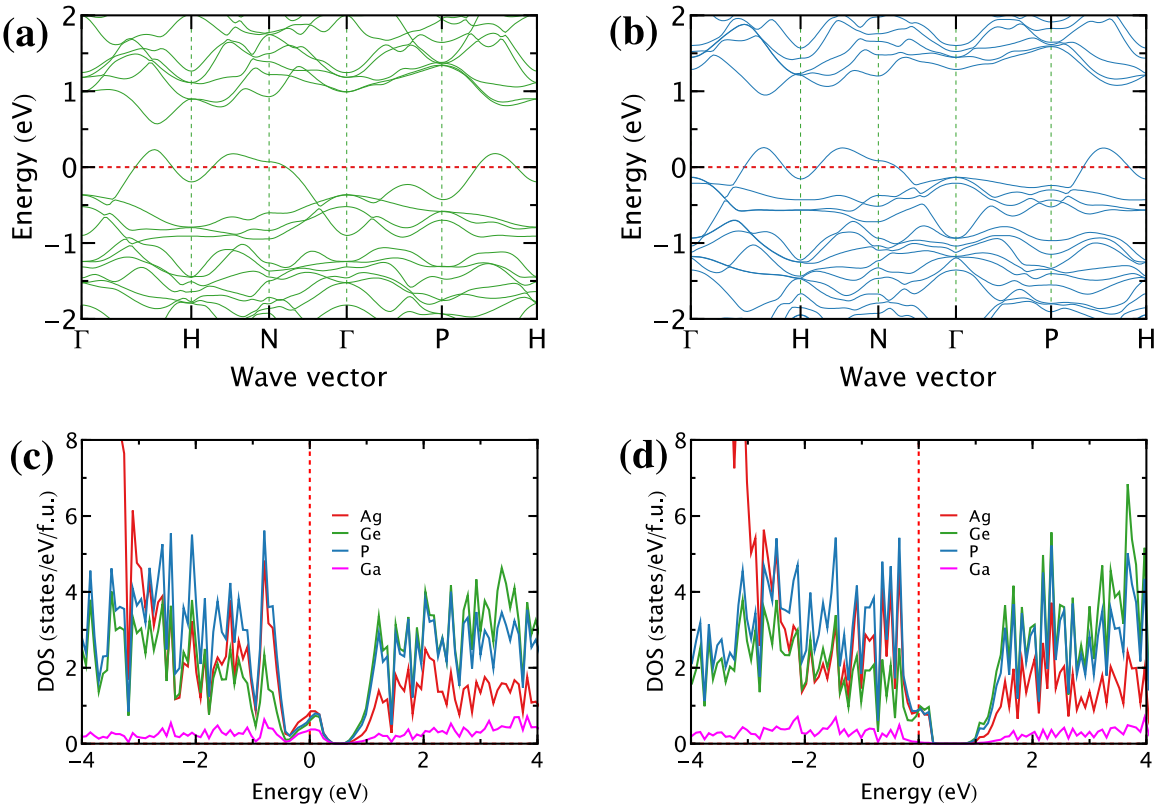

Fig. S4. (a) and (b) Band structure of $Ag_6Ge_9GaP_{12}$. (c) and (d) Atom-decomposed density of states $Ag_6Ge_9GaP_{12}$. In (a) and (c) Ga substitutes Ge(1), while in (b) and (d) Ga substitutes Ge(2). The dashed red line indicates the Fermi level.

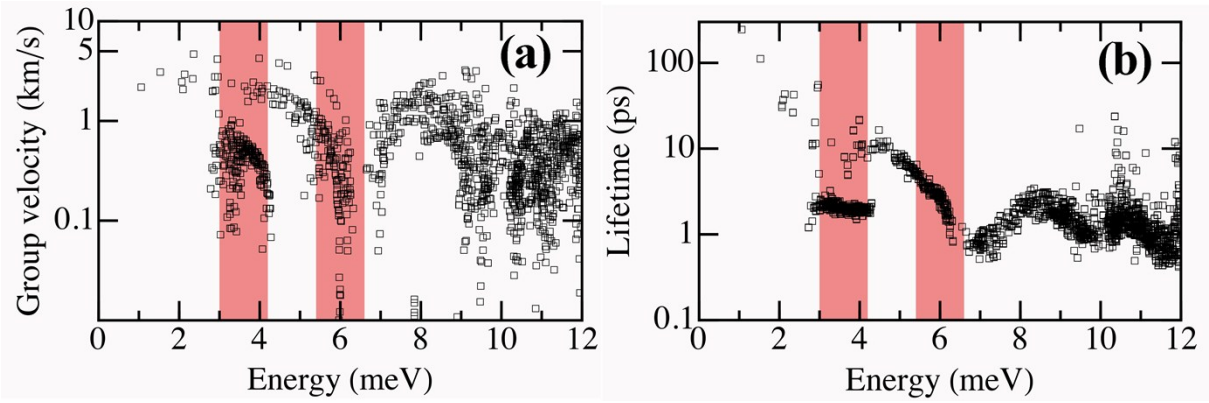

Fig. S5. (a) Calculated phonon mode group velocity; (b) Calculated phonon mode lifetime at 300 K.