Supporting Information

High Thermoelectric Performance in Complex Phosphides

Enabled by Stereochemically Active Lone Pair Electrons

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Fig. S1. Measured heat capacity of Ag₆Ge₁₀P₁₂.
Fig. S2. (a, b) SEM-EDX elemental mapping images of the surface of $\text{Ag}_6\text{Ge}_{9.7}\text{Ga}_{0.3}\text{P}_{12}$. 
Fig. S3. (a) Brillouin zone of the bcc unit cell of Ag$_6$Ge$_{10}$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$_6$Ge$_9$GaP$_{12}$. (c) and (d) Atom-decomposed density of states Ag$_6$Ge$_9$GaP$_{12}$. 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.