Supplementary Material for "Excellent Thermoelectric Performance in Alkali Metal Phosphides M_3P (M = Na and K) With Phonon-Glass Electron-Crystal Like Behaviour"

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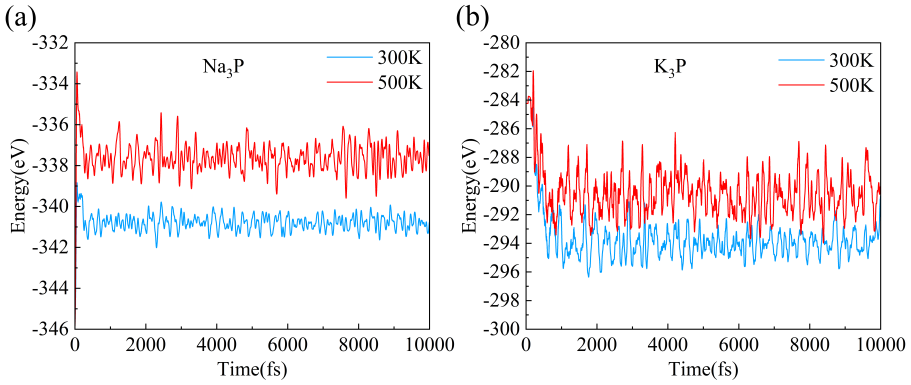

FIG. S1. The total energies of (a) Na_3P and (b) K_3P in the AIMD simulations at different temperatures.

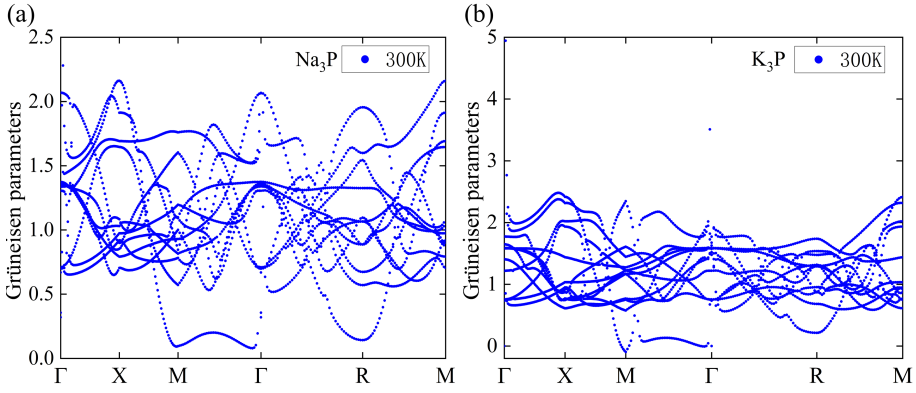

FIG. S2. The Grüneisen parameter for (a) Na_3P and (b) K_3P at 300K.

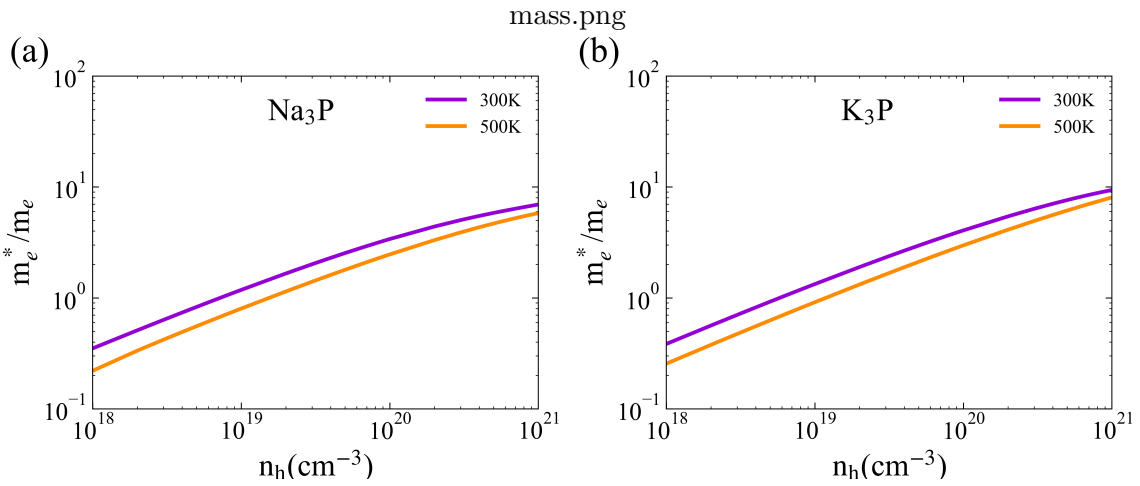

FIG. S3. The electron effective mass of (a) p-type doped Na_3P and (b) p-type doped K_3P at 300K and 500K.

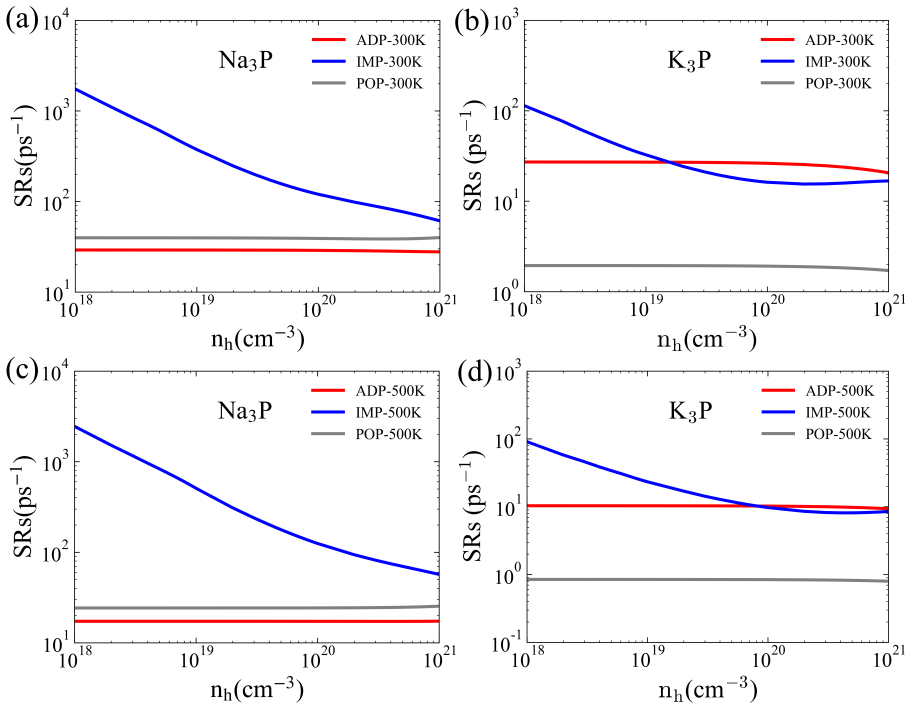

FIG. S4. The p-type doped electron scattering rates (SRs) of (a) Na_3P at 300K, (b) K_3P at 300K, (c)Na_3P at 500K, and (d) K_3P at 500K with different scattering mechanisms.

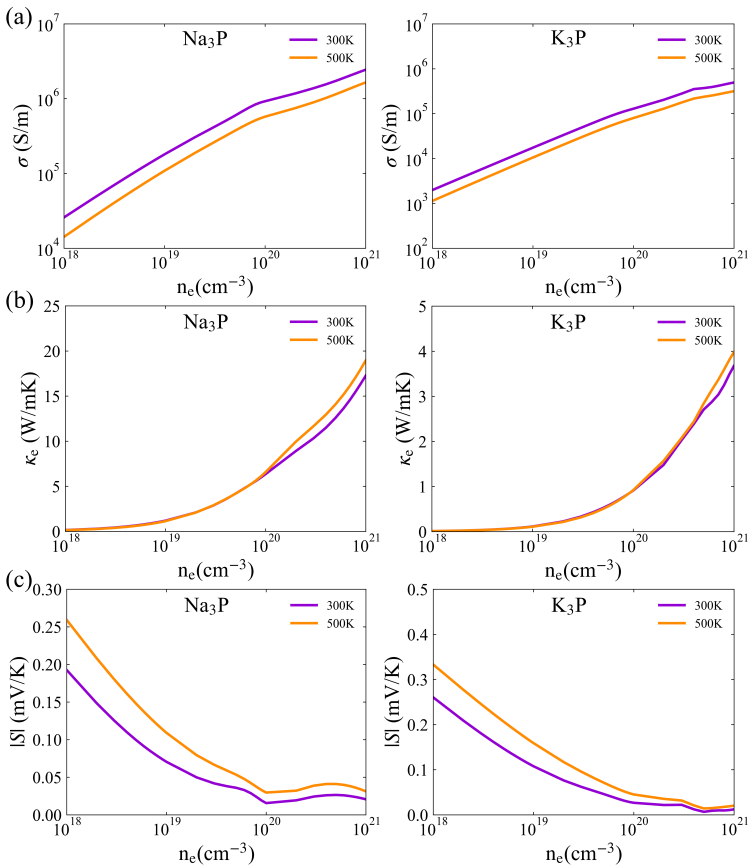

FIG. S5. The electronic transport parameters for n-type doping level ranging from 1.0×10^{18} to 1.0×10^{21}cm^{-3} at 300K and 500K. (a) Electrical conductivity for Na_3P (left) and K_3P (right). (b) Electrical thermal conductivity for Na_3P (left) and K_3P (right). (c) Seebeck coefficient for Na_3P (left) and K_3P (right).

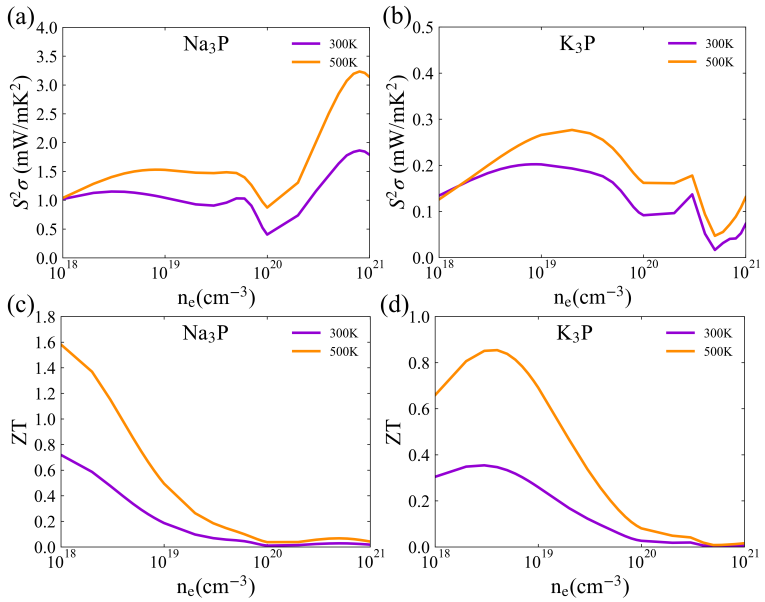

FIG. S6. The calculated Power factor PF and ZT for n-type doping level ranging from 1.0×10^{18} to $1.0\times\ 10^{21}\mathrm{cm}^{-3}$ at 300K and 500K: (a) PF of Na_3P, (b) PF of K_3P, (c) ZT of Na_3P and (d) ZT of K_3P.