Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information – Metal phosphide CuP_2 as a promising thermoelectric material: an insight from first-principles study*

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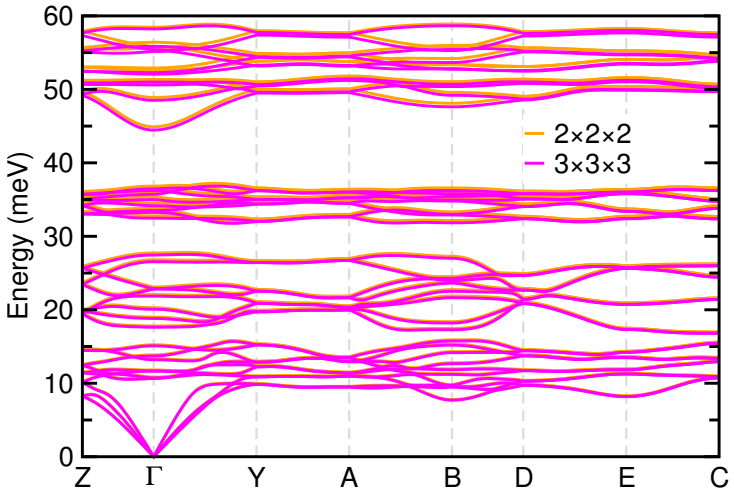

Figure S1. Comparison of harmonic phonon dispersion relations calculated using 2×2×2 (brown-colored lines) and 3×3×3 (pink-colored lines) supercells of monoclinic CuP_2 at 0 K.

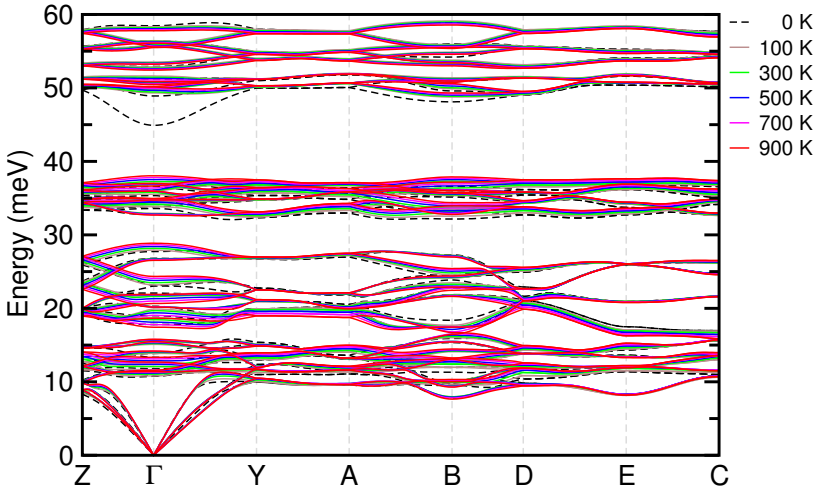

Figure S2. Temperature-dependent anharmonic phonon dispersion curves at different temperatures ranging from 100 to 900 K with an interval of 200 K, compared with harmonic ones for CuP_2.

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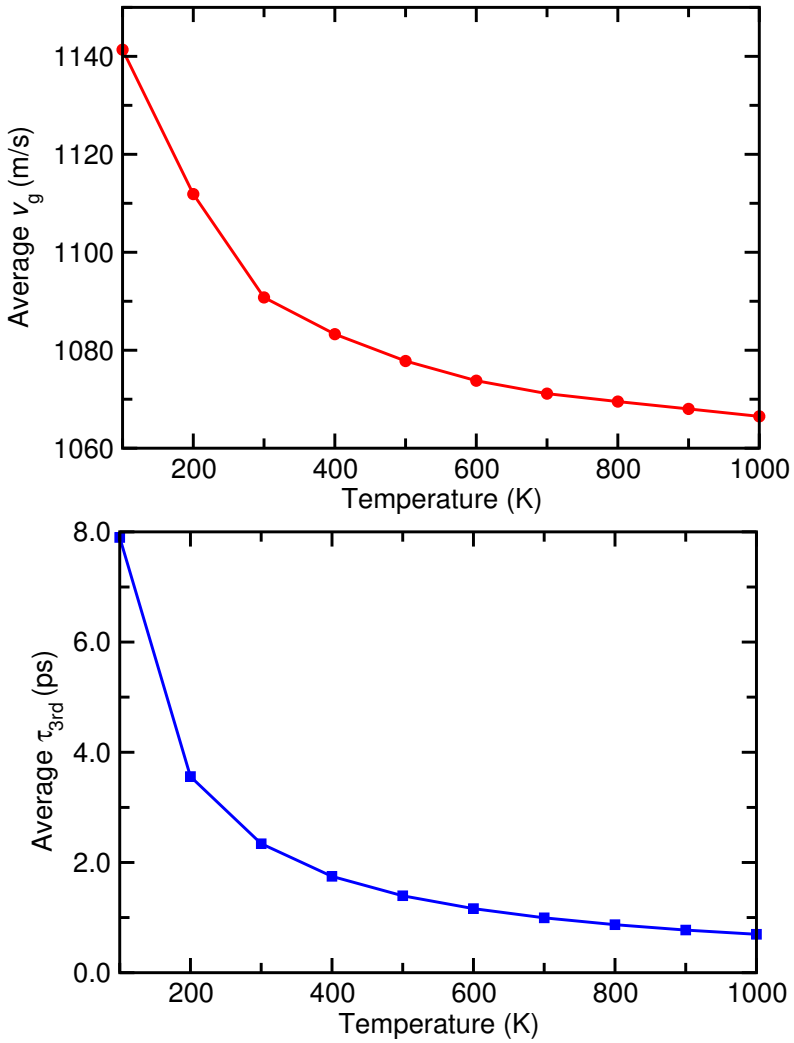

Figure S3. Average phonon lifetime τ_{rd} and group velocity v_g at temperatures from 100 to 1000 K with an interval of 100 K calculated with BTE+SCP method for CuP_2.

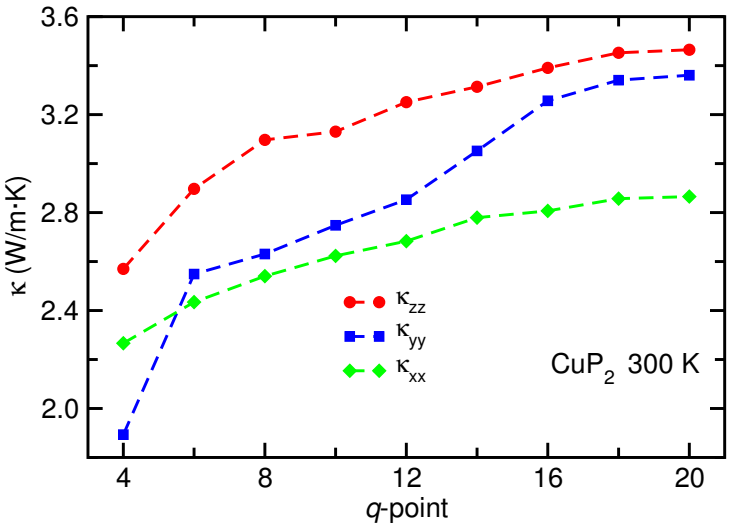

Figure S4. Convergence test for lattice thermal conductivity of CuP_2 according to the size of q-point mesh.

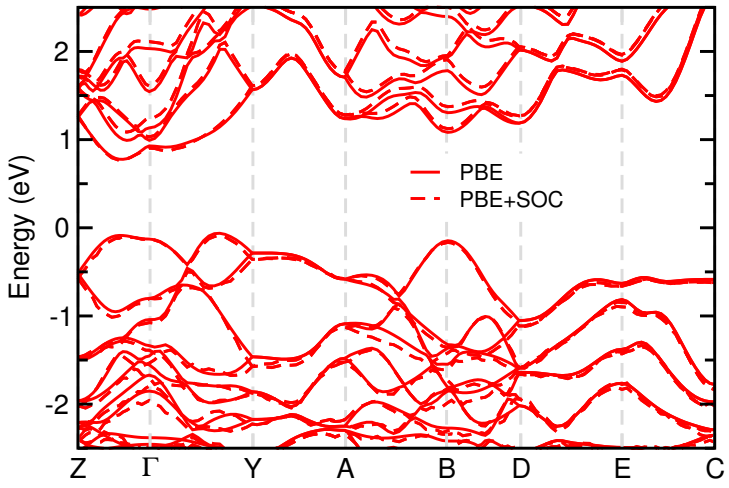

Figure S5. The PBE-calculated electronic band structures with and without the spin-orbit coupling (SOC) effect for CuP_2.

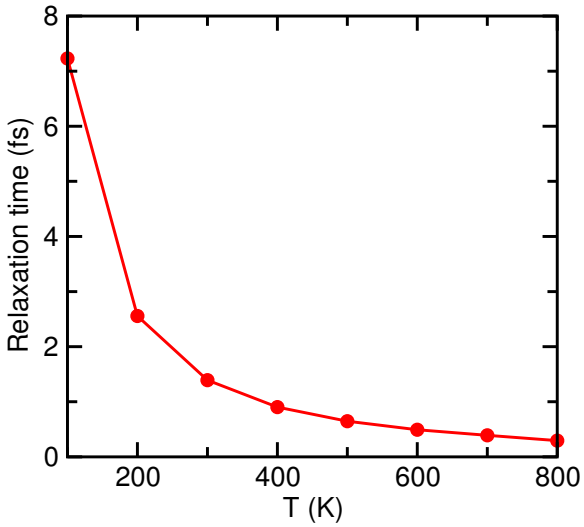

Figure S6. Relaxation time of electron as a function of temperature for CuP_2.

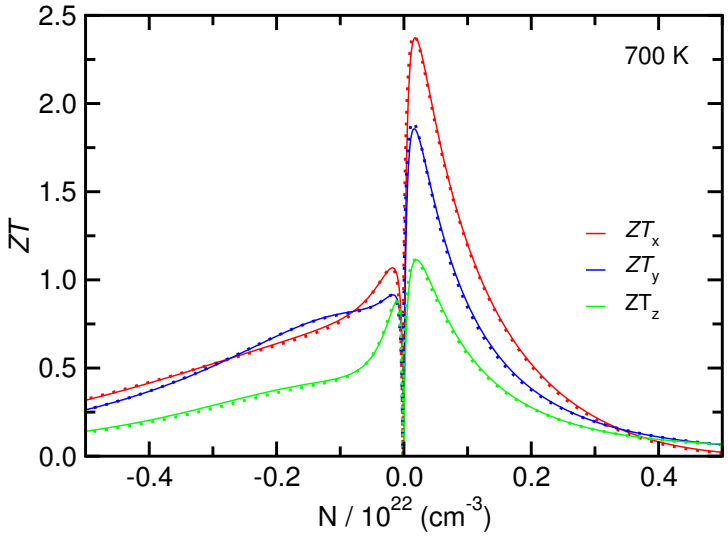

Figure S7. The PBE-calculated figure of merit ZT using k-point meshes of 24×24×16 (solid) and 20×20×12 (dotted) with relaxation time of 10^{-14} s for CuP_2.

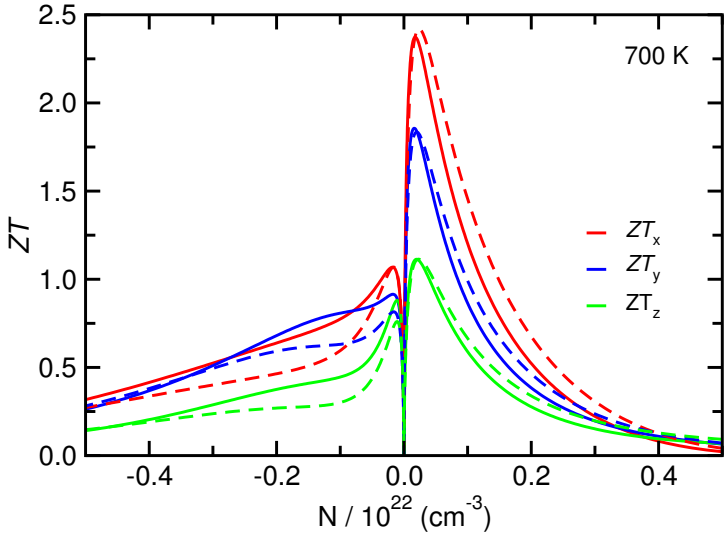

Figure S8. The figure of merit ZT calculated with the PBE (solid) and mBJ (dashed) functionals setting relaxation time to 10^{-14} s for CuP_2.