Anharmonicity-Driven low Lattice Thermal Conductivity and High Thermoelectric Response in Monolayer CeX_2 (X=O, S, Se, Te)

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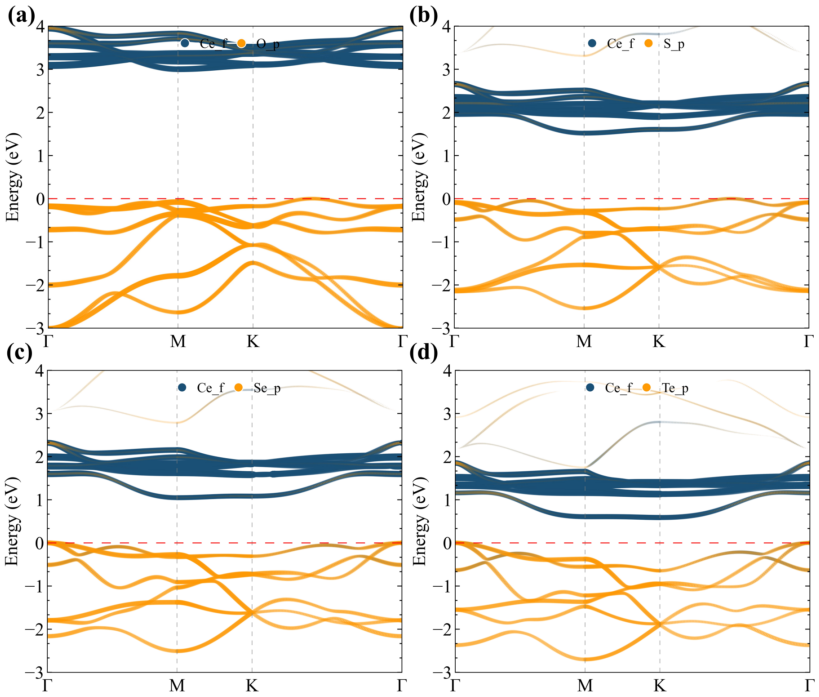

FIG. S1. Orbital-projected band structures of CeX_2.

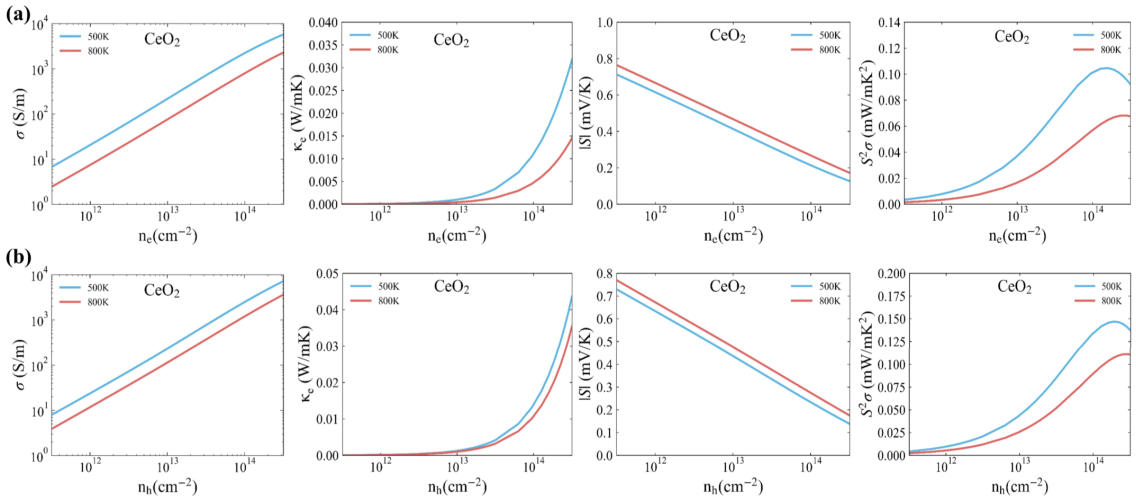

FIG. S2. The calculated electrical conductivity (σ), Seebeck coefficient (S), electronic thermal conductivity (κ_e) and power factor (PF = $S^2\sigma$) at 500 and 800 K without SOC for (a) n-type and (b) p-type CeO_2.

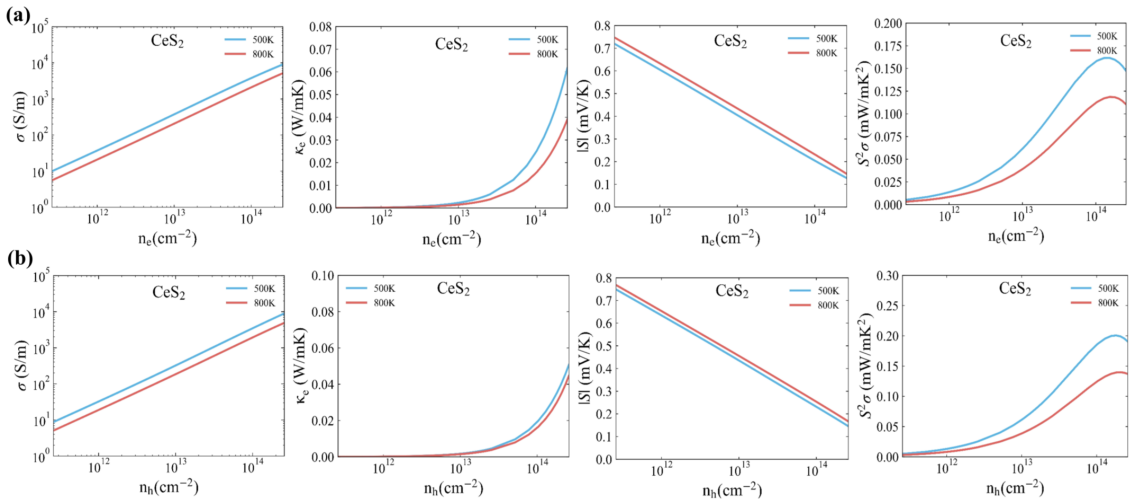

FIG. S3. The calculated electrical conductivity (σ), Seebeck coefficient (S), electronic thermal conductivity (κ_e) and power factor (PF = $S^2\sigma$) at 500 and 800 K without SOC for (a) n-type and (b) p-type CeS_2.

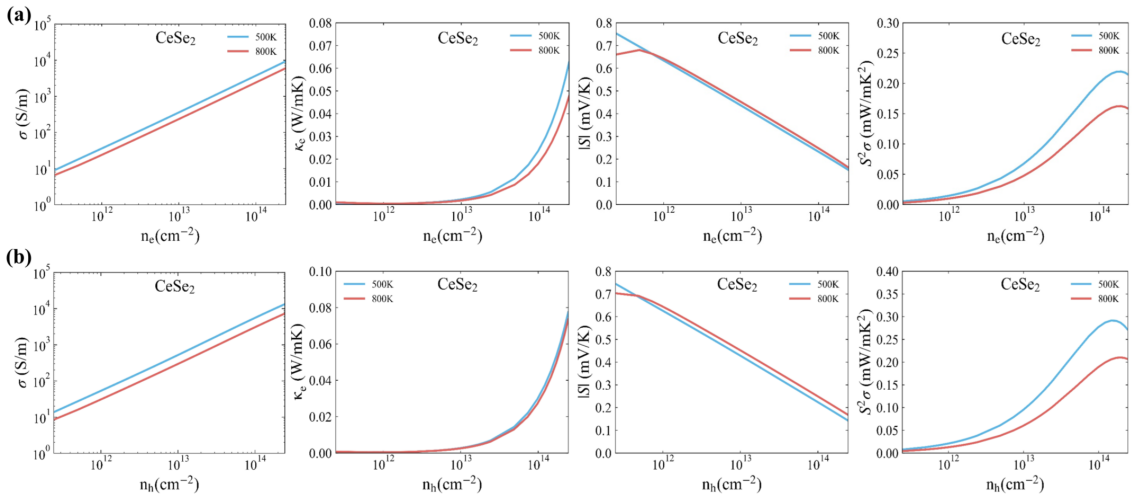

FIG. S4. The calculated electrical conductivity (σ), Seebeck coefficient (S), electronic thermal conductivity (κ_e) and power factor (PF = $S^2\sigma$) at 500 and 800 K without SOC for (a) n-type and (b) p-type $CeSe_2$.

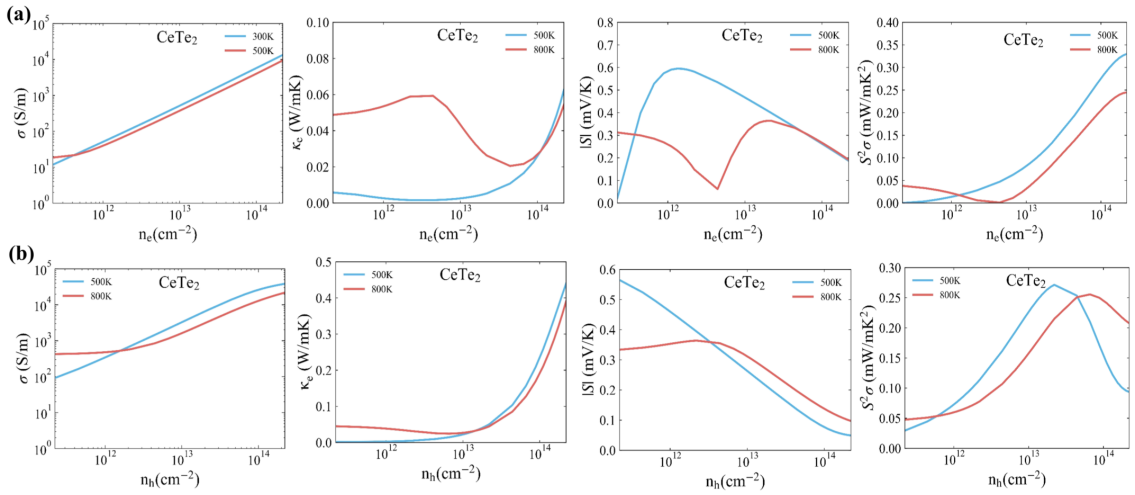

FIG. S5. The calculated electrical conductivity (σ), Seebeck coefficient (S), electronic thermal conductivity (κ_e) and power factor (PF = $S^2\sigma$) at 500 and 800 K without SOC for (a) n-type and (b) p-type $CeTe_2$.

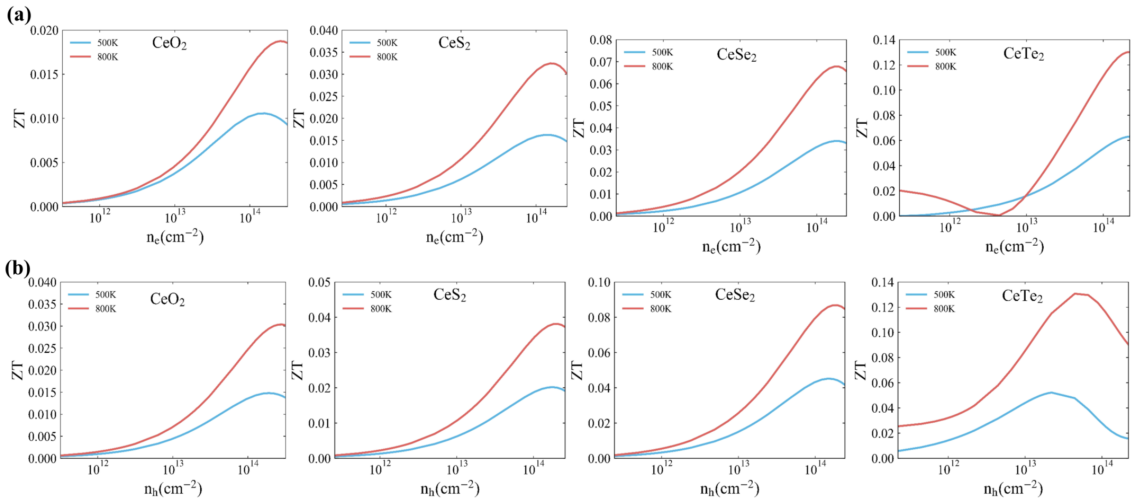

FIG. S6. The calculated ZT at 500 and 800 K without SOC for (a) n-type and (b) p-type CeX_2.

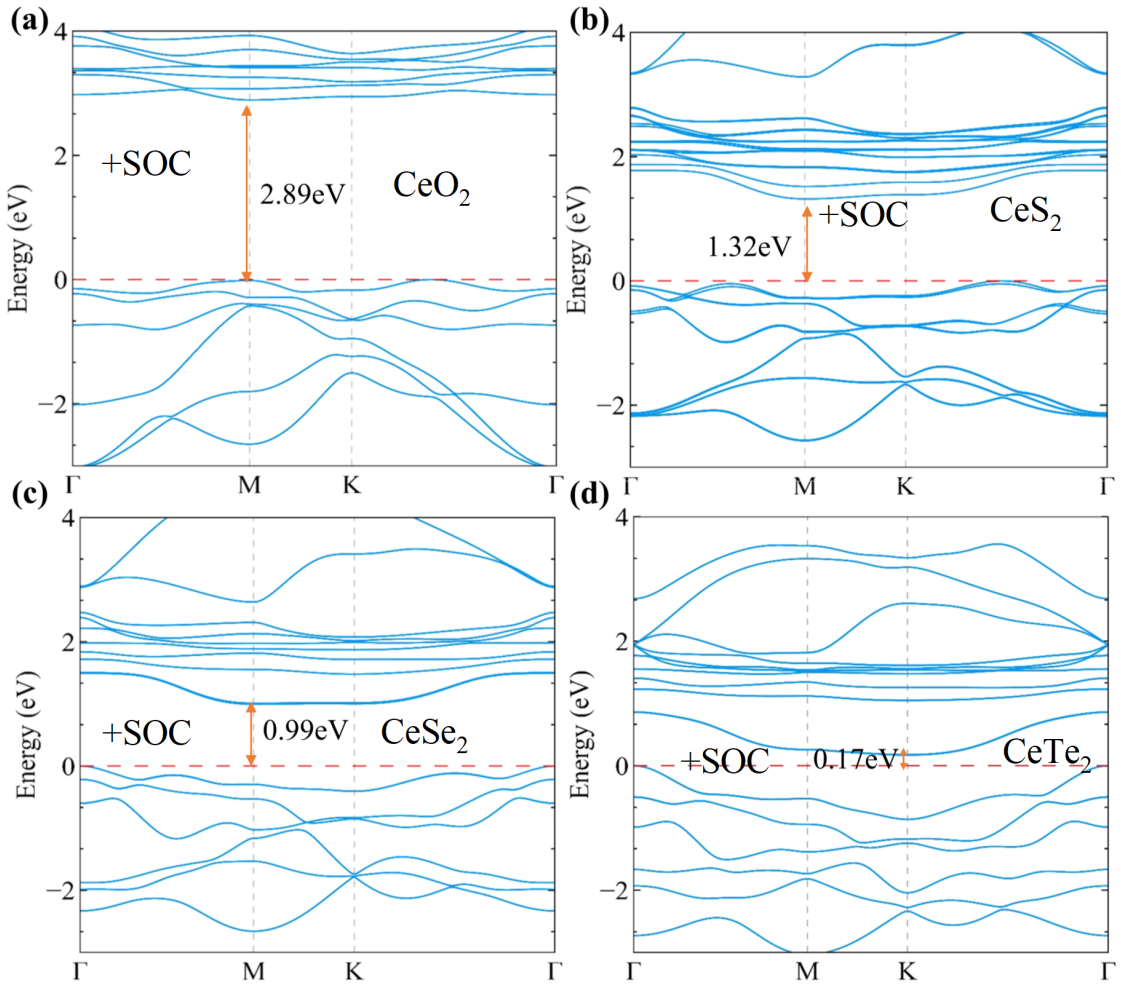

FIG. S7. The calculated band structures with SOC for (a) CeO_2, (b) CeS_2, (c) $CeSe_2$ and (d) $CeTe_2$.

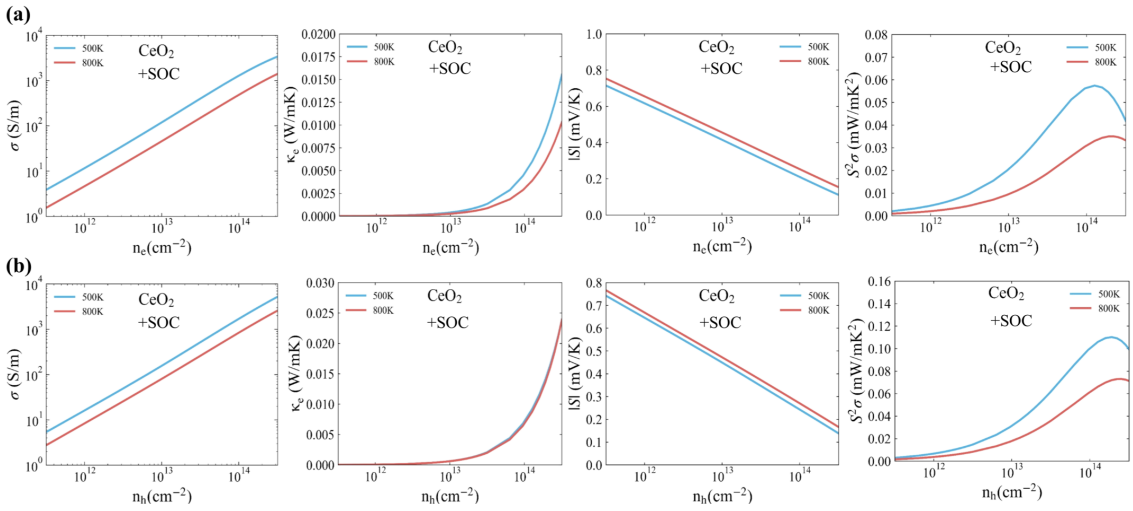

FIG. S8. The calculated electrical conductivity (σ), Seebeck coefficient (S), electronic thermal conductivity (κ_e) and power factor (PF = $S^2\sigma$) at 500 and 800 K with SOC for (a) n-type and (b) p-type CeO_2.

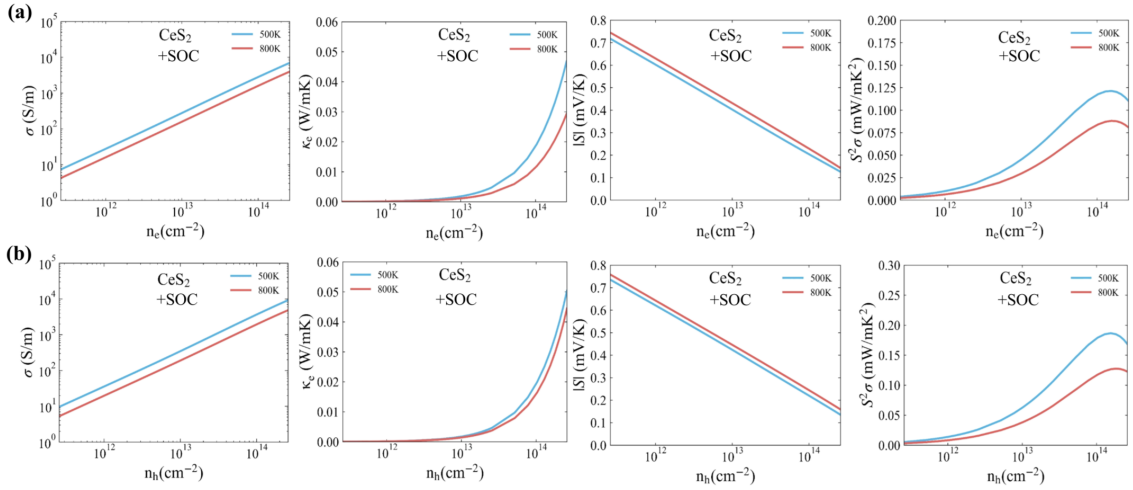

FIG. S9. The calculated electrical conductivity (σ), Seebeck coefficient (S), electronic thermal conductivity (κ_e) and power factor (PF = $S^2\sigma$) at 500 and 800 K with SOC for (a) n-type and (b) p-type CeS_2.

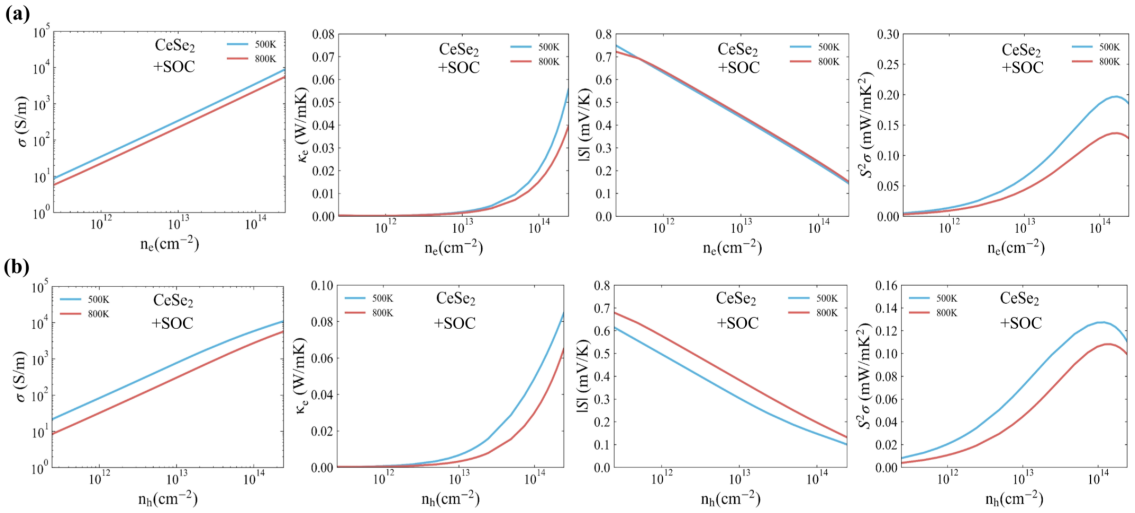

FIG. S10. The calculated electrical conductivity (σ), Seebeck coefficient (S), electronic thermal conductivity (κ_e) and power factor (PF = $S^2\sigma$) at 500 and 800 K with SOC for (a) n-type and (b) p-type $CeSe_2$.

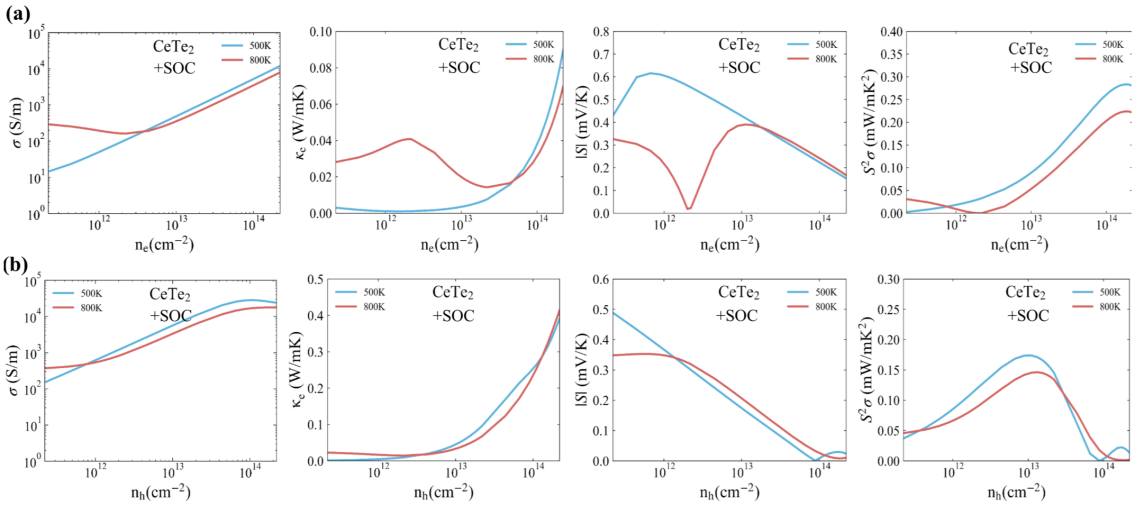

FIG. S11. The calculated electrical conductivity (σ), Seebeck coefficient (S), electronic thermal conductivity (κ_e) and power factor (PF = $S^2\sigma$) at 500 and 800 K with SOC for (a) n-type and (b) p-type $CeTe_2$.

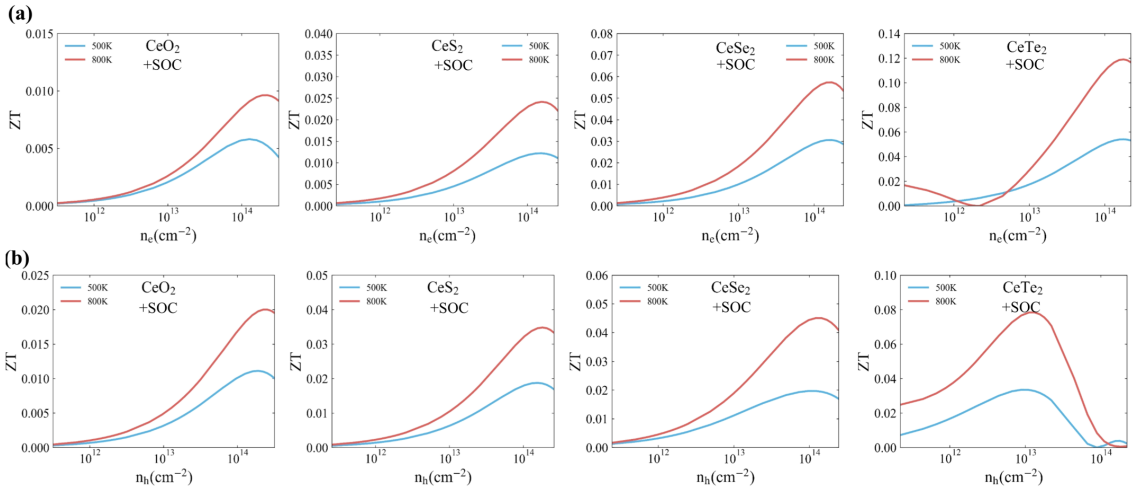

FIG. S12. The calculated ZT at 500 and 800 K with SOC for (a) n-type and (b) p-type CeX_2.

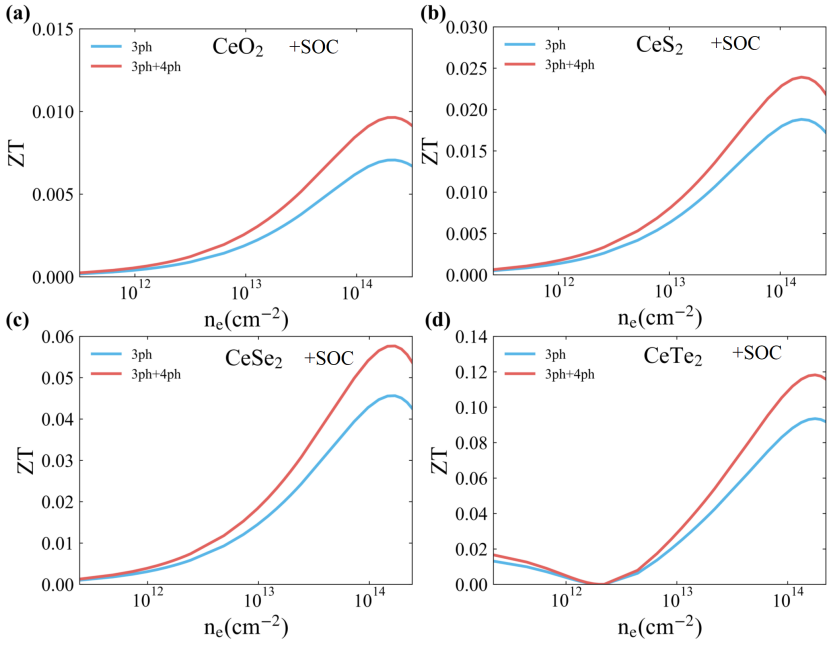

FIG. S13. The calculated ZT at 800 K for n-type (a) CeO_2, (b) CeS_2, (c) $CeSe_2$ and (d) $CeTe_2$ with and without 4ph scattering.

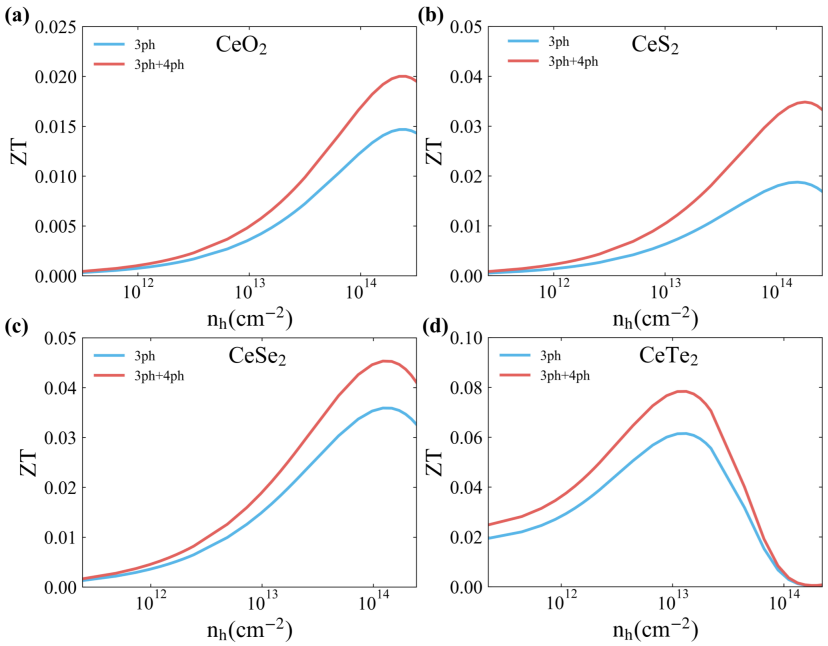

FIG. S14. The calculated ZT at 800 K for p-type (a) CeO_2, (b) CeS_2, (c) $CeSe_2$ and (d) $CeTe_2$ with and without 4ph scattering.