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Synergistic Effects of K-Atom Rattling, Anisotropy, and Antibonding States on High Thermoelectric Performance in $KAuSe_2$

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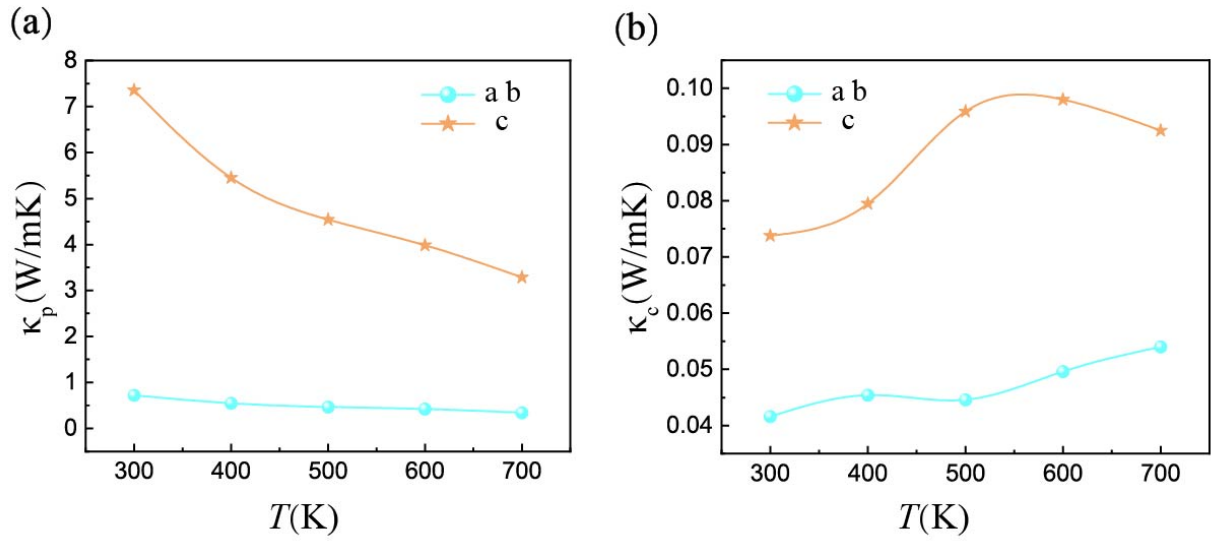

Figure 1: Calculated temperature-dependent (a)κ_p , (b)κ_c considering 3+4ph scattering along different directions.

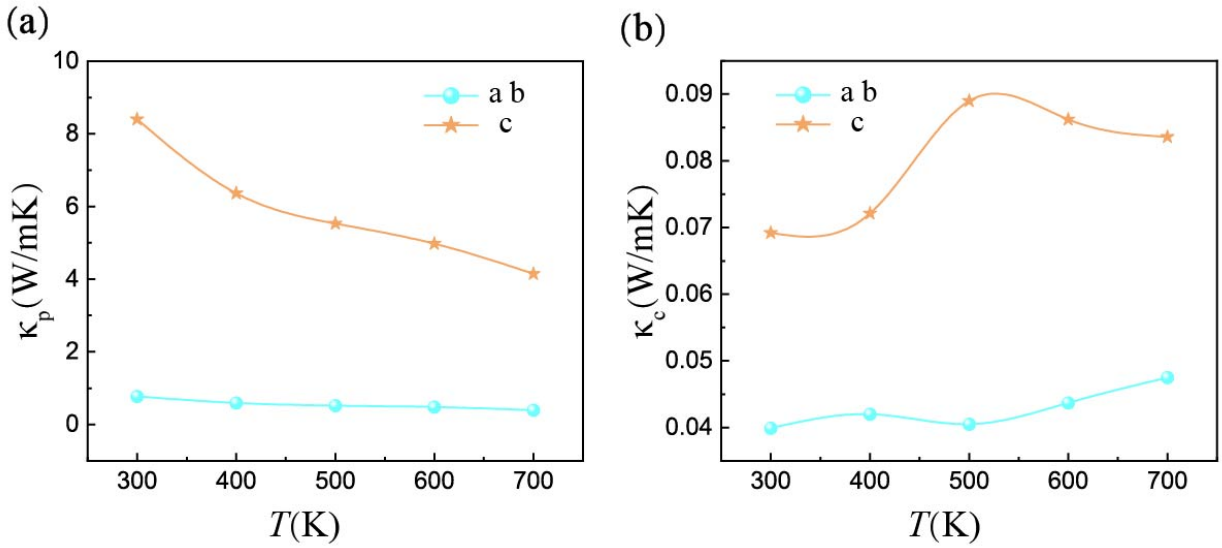

Figure 2: Calculated temperature-dependent (a)κ_p , (b)κ_c considering 3ph scattering along different directions.

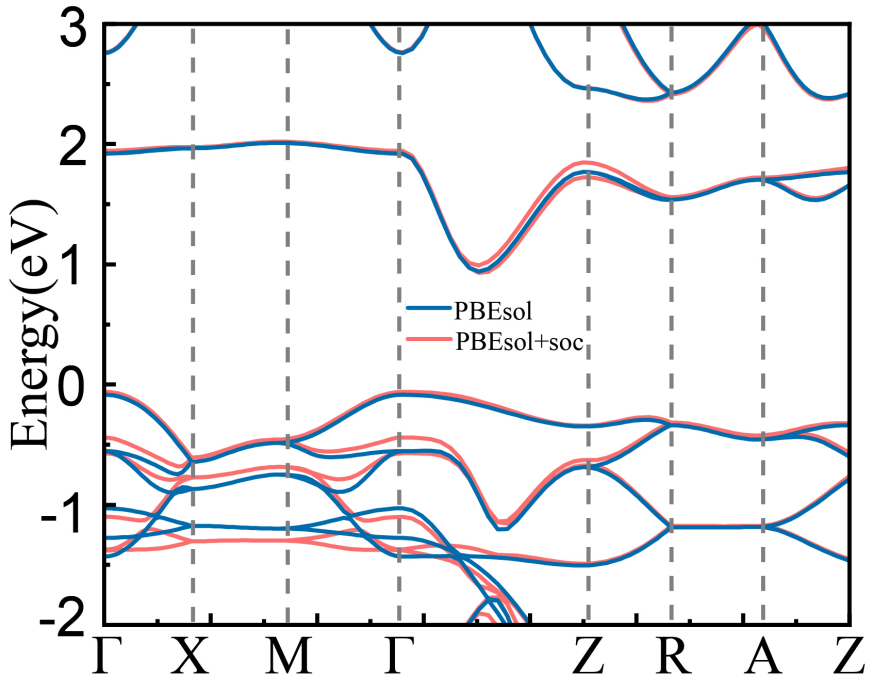

Figure 3: Comparison of PBEsol (blue line) and PBEsol+SOC (red line) electronic band structures.