

# Electronic Supplementary Information (ESI) – Theoretical insights into lattice dynamics and transport properties for lead-free quadruple halide perovskite $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$

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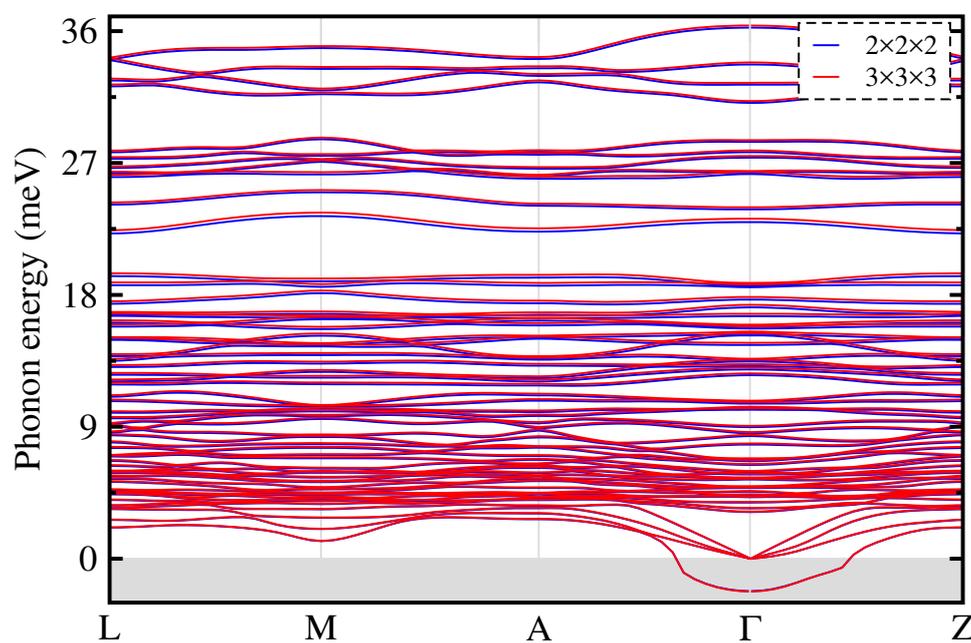


Fig. S1 Convergence tests of the harmonic phonon dispersion curves according to the supercell size for the quadruple halide perovskite  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  with the monoclinic  $C2/m$  space group.

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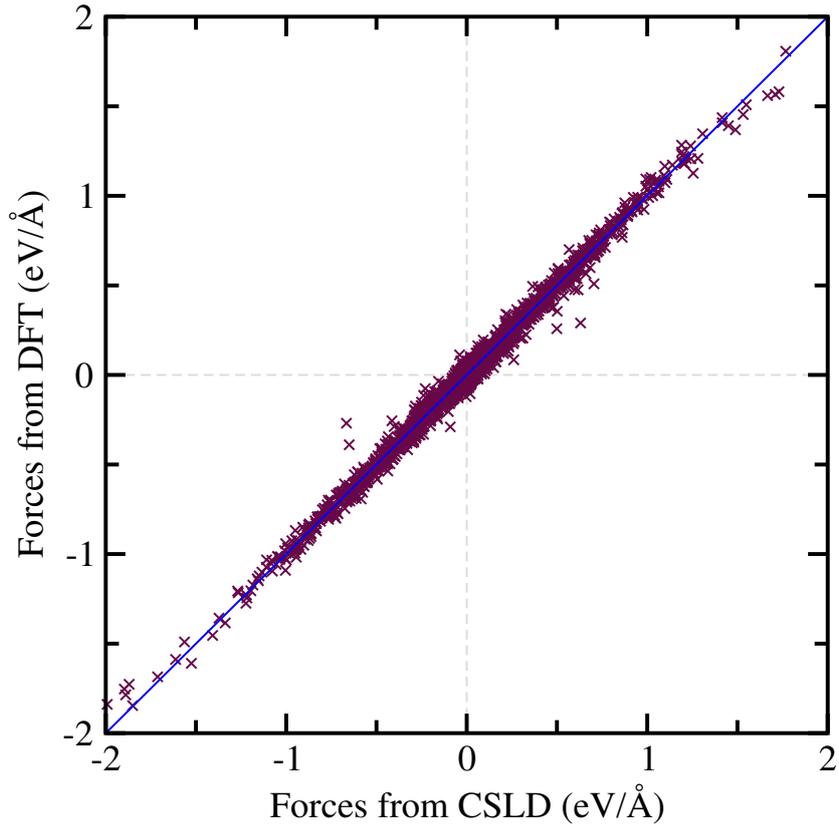


Fig. S2 Comparison of the atomic forces obtained from the DFT and CSLD calculations for the quadruple halide perovskite  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  with the monoclinic  $C2/m$  space group.

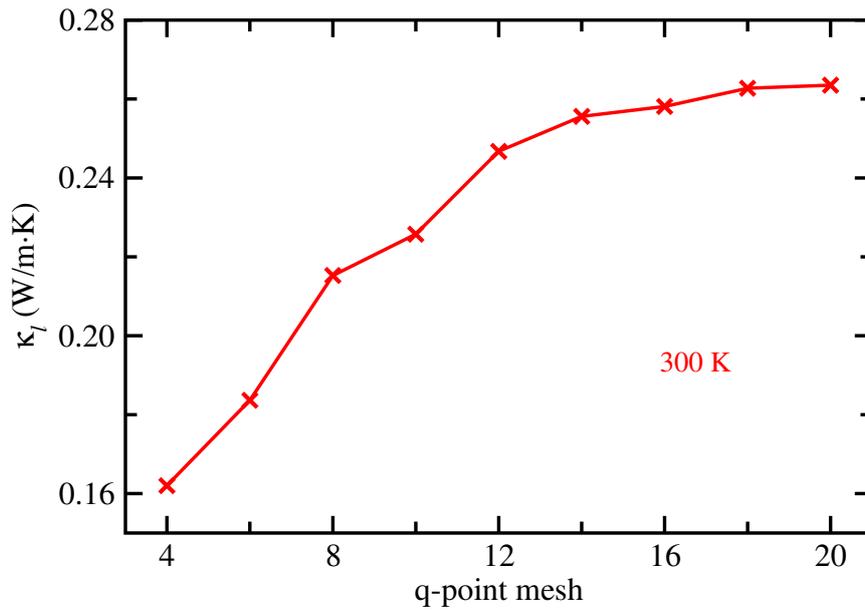


Figure S3 Convergence test of the lattice thermal conductivity  $\kappa_l$  according to the size of the  $q$ -point mesh for the quadruple halide perovskite  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  with the monoclinic  $C2/m$  space group.

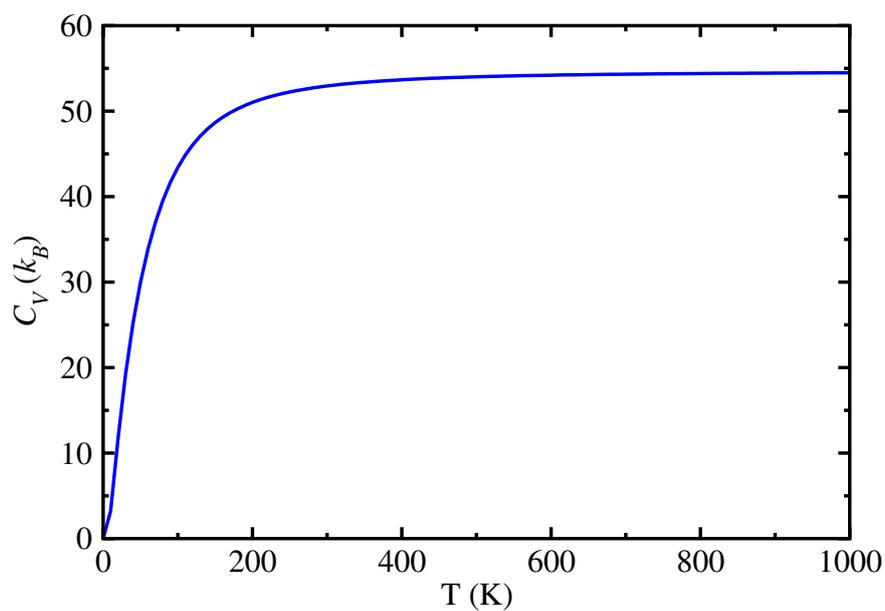


Figure S4 Heat capacity  $C_V$  calculated as a function of temperature for the quadruple halide perovskite  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  with the monoclinic  $C2/m$  space group.

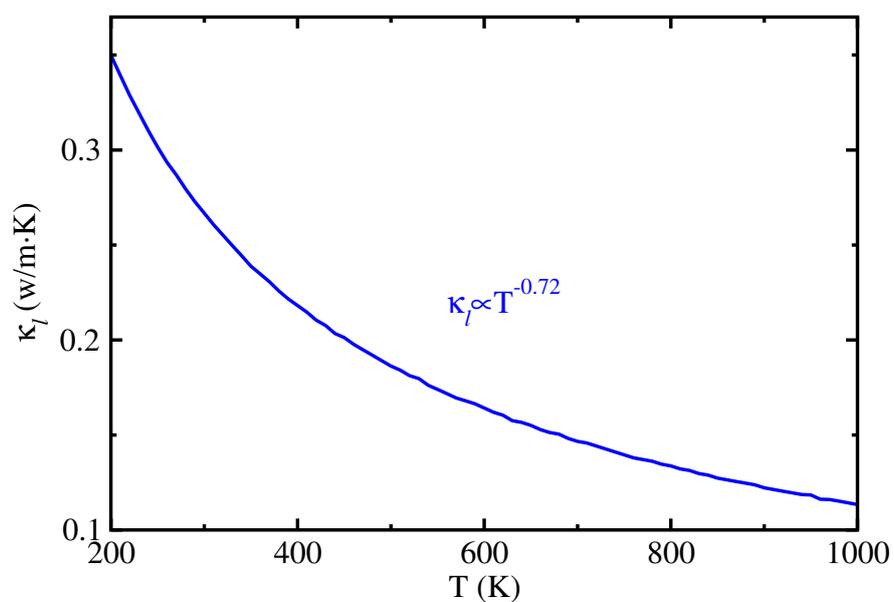


Figure S5 Average lattice thermal conductivity  $\kappa_l$  as a function of temperature for the quadruple halide perovskite  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  with the monoclinic  $C2/m$  space group.

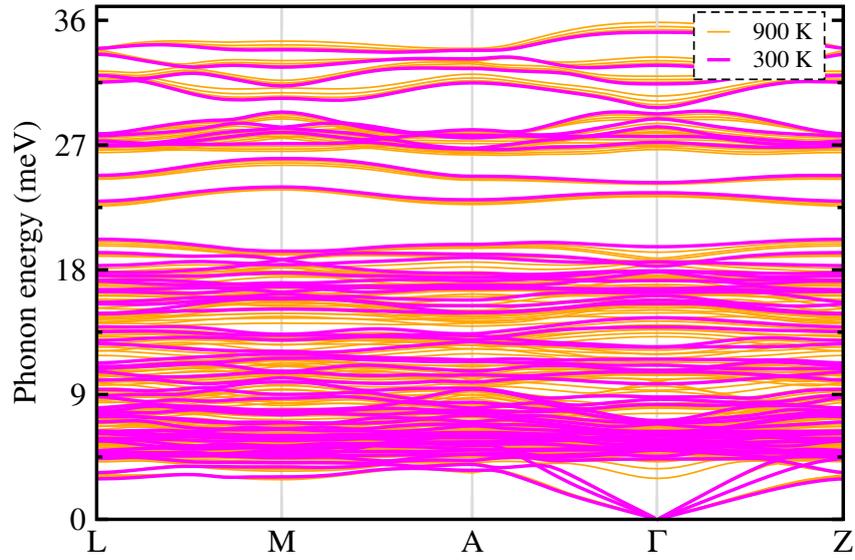


Figure S6 Self-consistent phonon dispersion curves calculated at temperatures from 300 K to 900 K with an interval of 200 K for the quadruple halide perovskite  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  with the monoclinic  $C2/m$  space group.

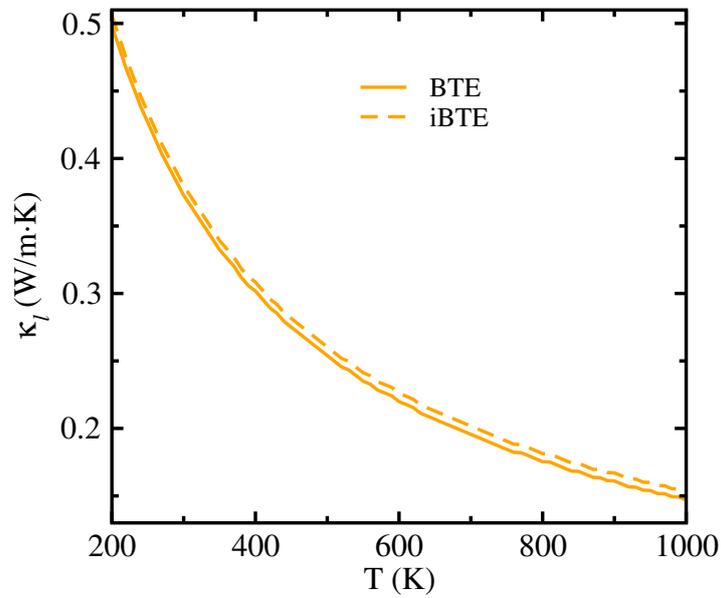


Figure S7 Comparison of lattice thermal conductivities calculated by iteratively (dashed) and non-iteratively (solid) solving the Boltzmann transport equation for the quadruple halide perovskite  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  with the monoclinic  $C2/m$  space group.