

Supplementary Information

Microscopic origin of the extremely low thermal conductivity and outstanding thermoelectric performance of BiSbX_3 ($\text{X}=\text{S}, \text{Se}$) revealed by first-principles study

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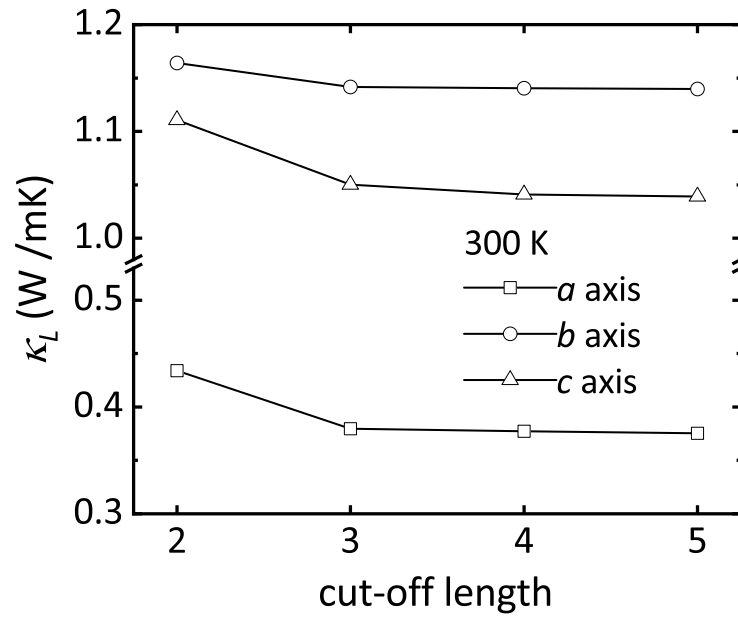


Fig. S1: The convergence tests for the cutoff interactions of nearest neighbors in the third-order IFCs (BiSbSe₃ at 300K).

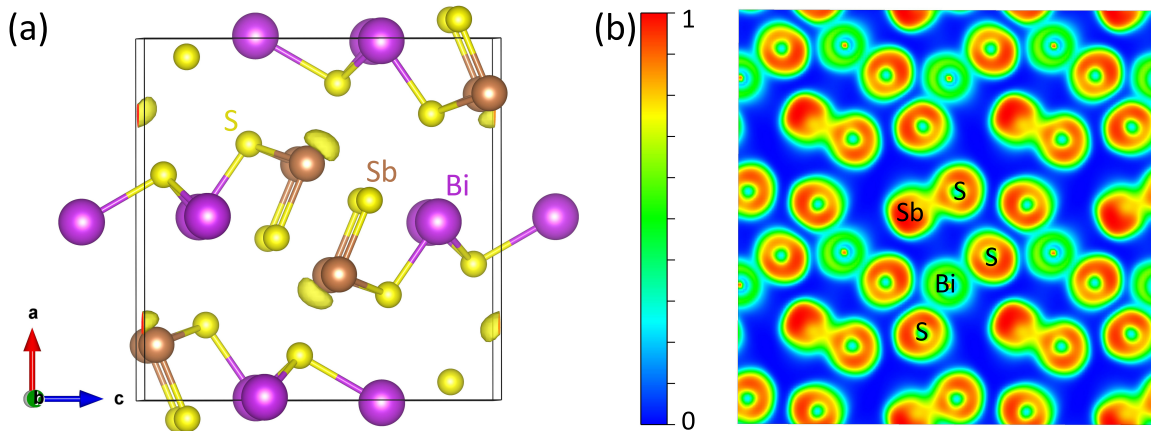


Fig. S2: (a) Calculated 3D ELF for BiSbS₃. The isosurface level is 0.93. (b) The projected ELF of BiSbS₃ onto the (010) plane.

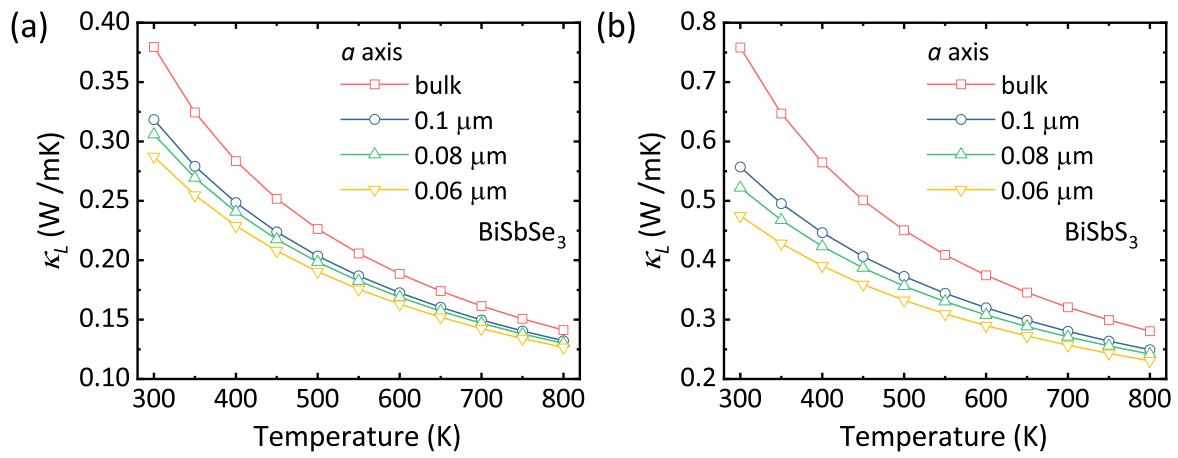


Fig. S3: The lattice thermal conductivities of infinite and finite size (0.1, 0.08, and 0.06 μm) for (a) BiSbSe_3 and (b) BiSbS_3 as a function of temperature.