ELECTRONIC SUPPLEMENTARY INFORMATION

One-dimensional van der Waals BiSBr: An Anisotropic Thermoelectric Mineral

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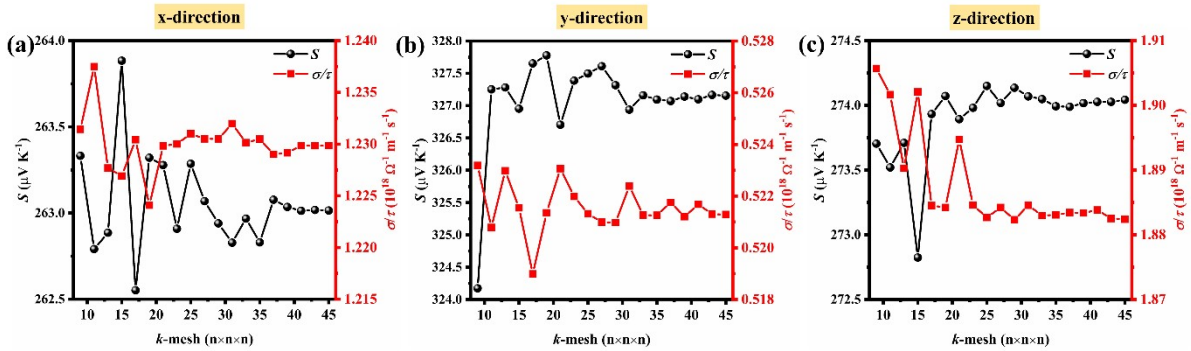

Fig. S1 Convergence test for *k*-mesh to calculate transport coefficients.

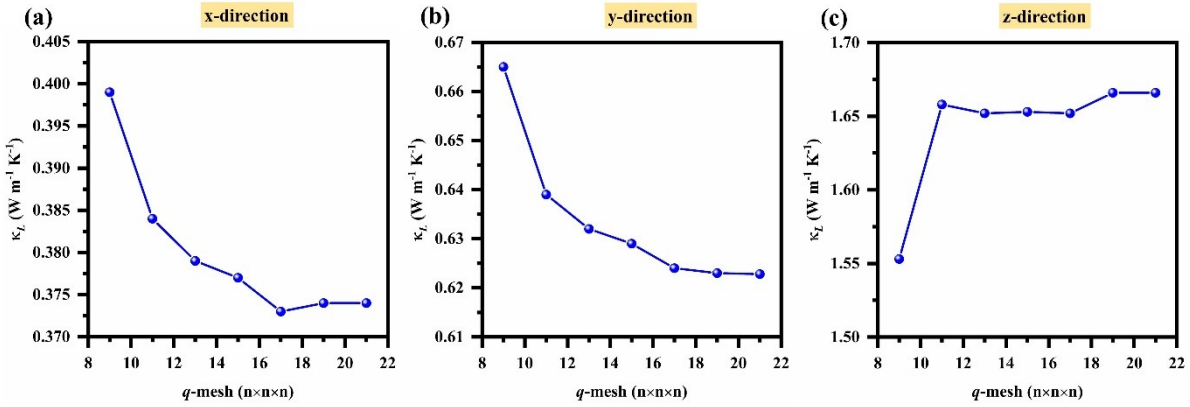

Fig. S2 Convergence test for κ-mesh to calculate lattice thermal conductivity.

Table ST1 The lattice parameters calculated with different functionals are compared with experimental report.

	Lattice parameters (Å)		
	a	***b***	***c***
PBE	8.158 **(+1.72 %)**	11.597 **(+19.55 %)**	4.061 **(+1.27 %)**
PBE+D3	8.153 **(+1.66 %)**	9.727 **(+0.28 %)**	4.051 **(+1.02 %)**
Expt. (Ref. 52)	8.020	9.700	4.010

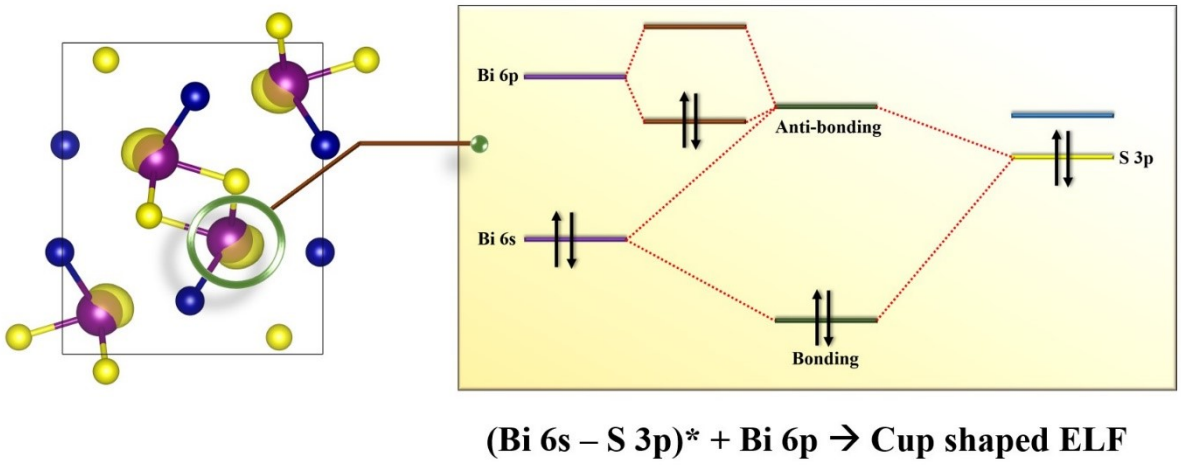

Fig. S3 3D ELF and the formation of cup-shaped ELF

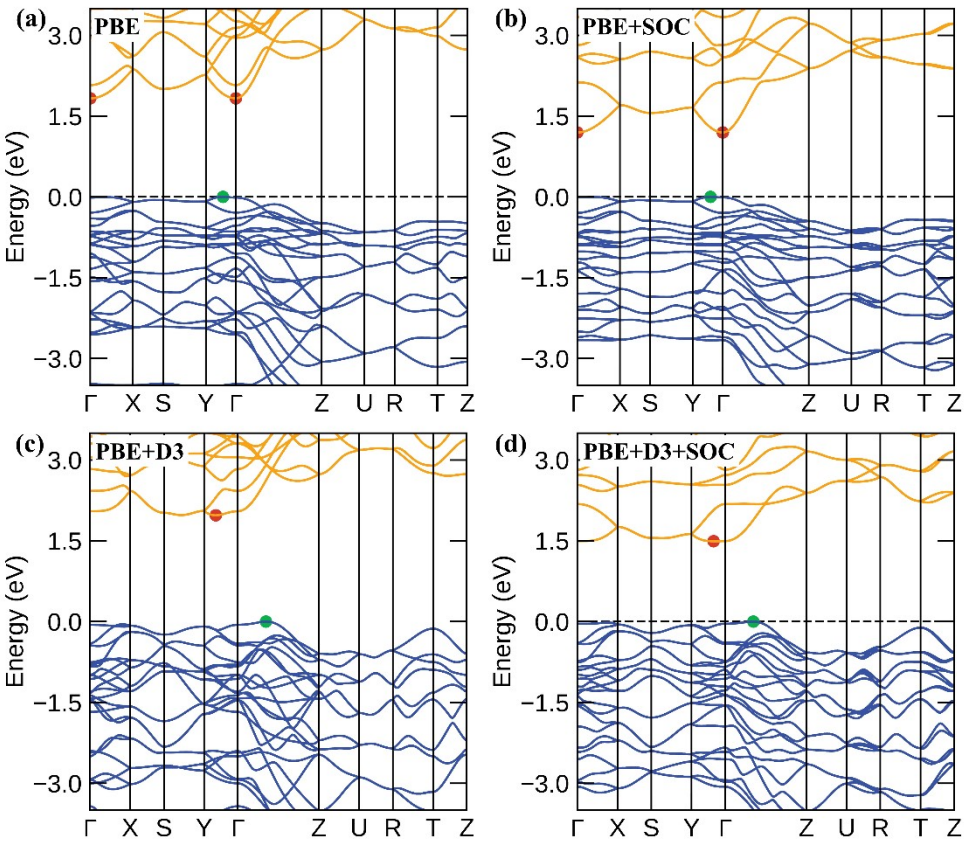

Figure S4 The effect of spin-orbit coupling and van der Waals corrections on the electronic band structure of BiSBr.

Table ST2 band gaps calculated with various functionals are listed against the experimental report

	E_g (eV)
PBE	1.83 **(-8.95 %)**
PBE+SOC	1.20 **(-40.30 %)**
PBE+D3	1.97 **(-1.99 %)**
PBE+D3+SOC	1.49 **(-25.87 %)**
Expt. (Ref. 52)	2.01

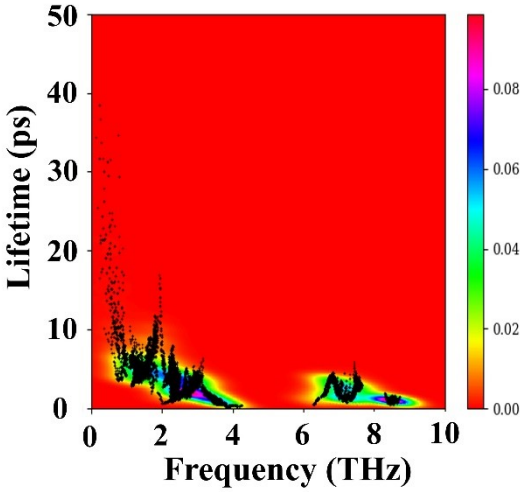

Fig. S5 Phonon lifetime as a function of frequency at 300 K