Supplementary information: First-principles study of thermal transport properties in ferroelectric HfO_2 and related fluorite-structure ferroelectrics

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Table. S1. The elastic constants (in units of GPa) for fluorite-structure ferroelectrics.

	C_{11}	C_{12}	C_{13}	C_{21}	C_{22}	C_{23}	C_{31}	C_{32}	C_{33}	C_{44}	C_{55}	C_{66}
ZrO_2	37.2	14.8	11.4	14.8	37.9	12.7	11.4	12.7	36.6	8.4	8.7	12.3
ZrS_2	19.7	7.0	6.8	7.0	13.4	5.5	6.8	5.5	14.1	2.5	4.0	6.5
$ZrSe_2$	16.3	5.8	5.5	5.8	11.3	4.7	5.5	4.7	11.8	1.8	2.6	5.4
HfO_2	39.3	15.3	11.8	15.3	40.9	13.2	11.8	13.2	40.0	9.3	9.5	13.6
HfS_2	20.9	7.2	6.5	7.2	15.1	5.7	6.5	5.7	16.5	2.9	3.8	6.8
$HfSe_2$	17.2	6.0	5.4	6.0	13.1	4.9	5.4	4.9	14.2	2.2	2.8	5.6
$CaCl_2$	6.6	2.9	2.0	2.9	5.7	1.9	2.0	1.9	6.2	1.4	1.5	2.1
$CaBr_2$	5.3	2.3	1.4	2.3	4.6	1.4	1.4	1.4	5.2	1.0	1.1	1.7
CaI_2	4.0	1.7	0.9	1.7	3.7	1.0	0.9	1.0	4.4	0.7	0.8	1.4
$SrCl_2$	5.4	2.6	2.1	2.6	4.5	1.7	2.1	1.7	4.1	1.2	1.3	1.8
$SrBr_2$	4.6	2.2	1.7	2.2	3.5	1.3	1.7	1.3	3.6	0.9	1.1	1.5
SrI_2	3.8	1.7	1.3	1.7	2.8	0.9	1.3	0.9	3.2	0.7	0.8	1.2

Table. S2. The elastic stability criteria for fluorite-structure ferroelectrics.

Criteria / Structure	(i)	(ii)	(iii)	(iv)	(v)	(vi)
ZrO_2	37.2	1190.8	36944.8	8.4	8.7	12.3
ZrS_2	19.7	215.0	2339.3	2.5	4.0	6.5
$ZrSe_2$	16.3	150.6	1374.5	1.8	2.6	5.4
HfO_2	39.3	1373.3	47154.9	9.3	9.5	13.6
HfS_2	20.9	263.8	3568.4	2.9	3.8	6.8
$HfSe_2$	17.2	189.3	2210.9	2.2	2.8	5.6
$CaCl_2$	6.6	29.2	156.5	1.4	1.5	2.1
$CaBr_2$	5.3	19.1	88.9	1.0	1.1	1.7
CaI_2	4.0	11.9	48.5	0.7	0.8	1.4
$SrCl_2$	5.4	17.5	55.0	1.2	1.3	1.8
$SrBr_2$	4.6	11.3	32.4	0.9	1.1	1.5
SrI_2	3.8	7.8	21.0	0.7	0.8	1.2

Criteria (i): $C_{11} > 0$; (ii): $C_{11}C_{22} - C_{12}^2 > 0$;

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(iii): $C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} - C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2 > 0$;

(iv): $C_{44} > 0$; (v): $C_{55} > 0$; (vi): $C_{66} > 0$.

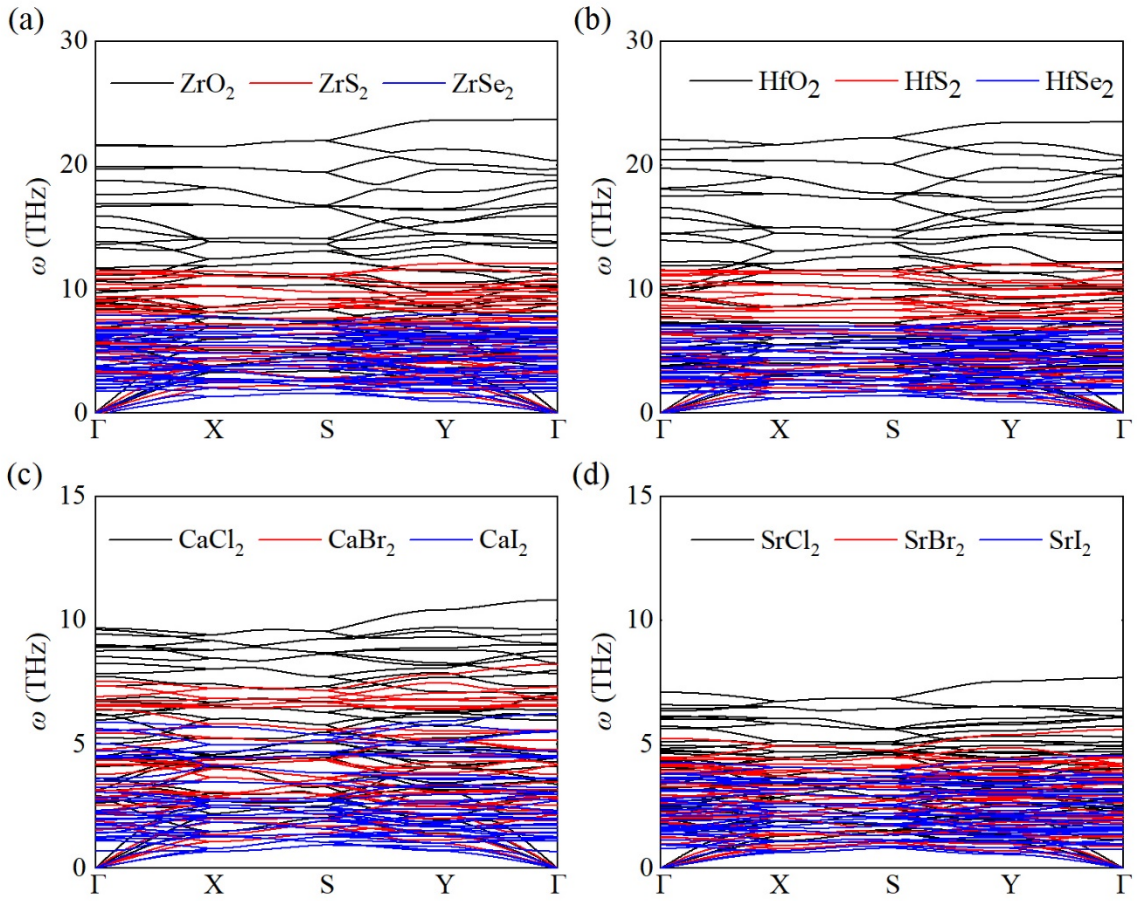

Fig. S1. The phonon dispersion curves for (a,b) group IV-VI and (c,d) group II-VII fluorite-structure ferroelectrics.

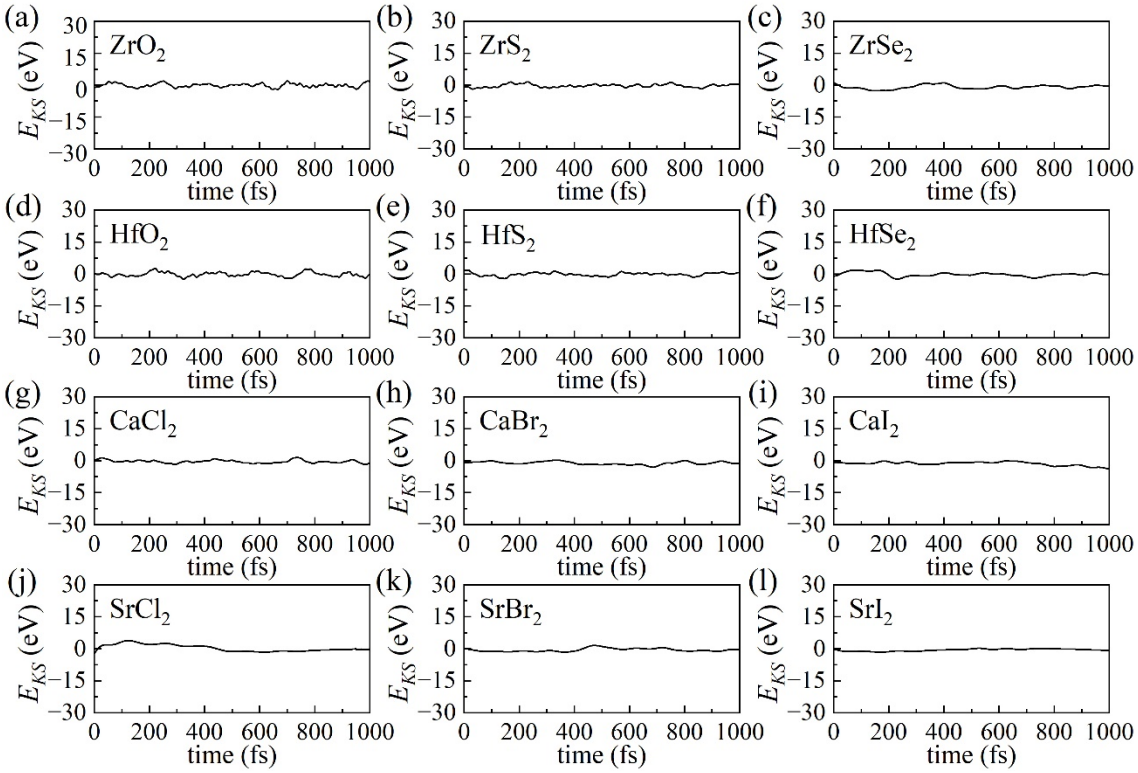

Fig. S2. *Ab-initio* molecular dynamics (AIMD) simulations at 300 K for fluorite-structure ferroelectrics.

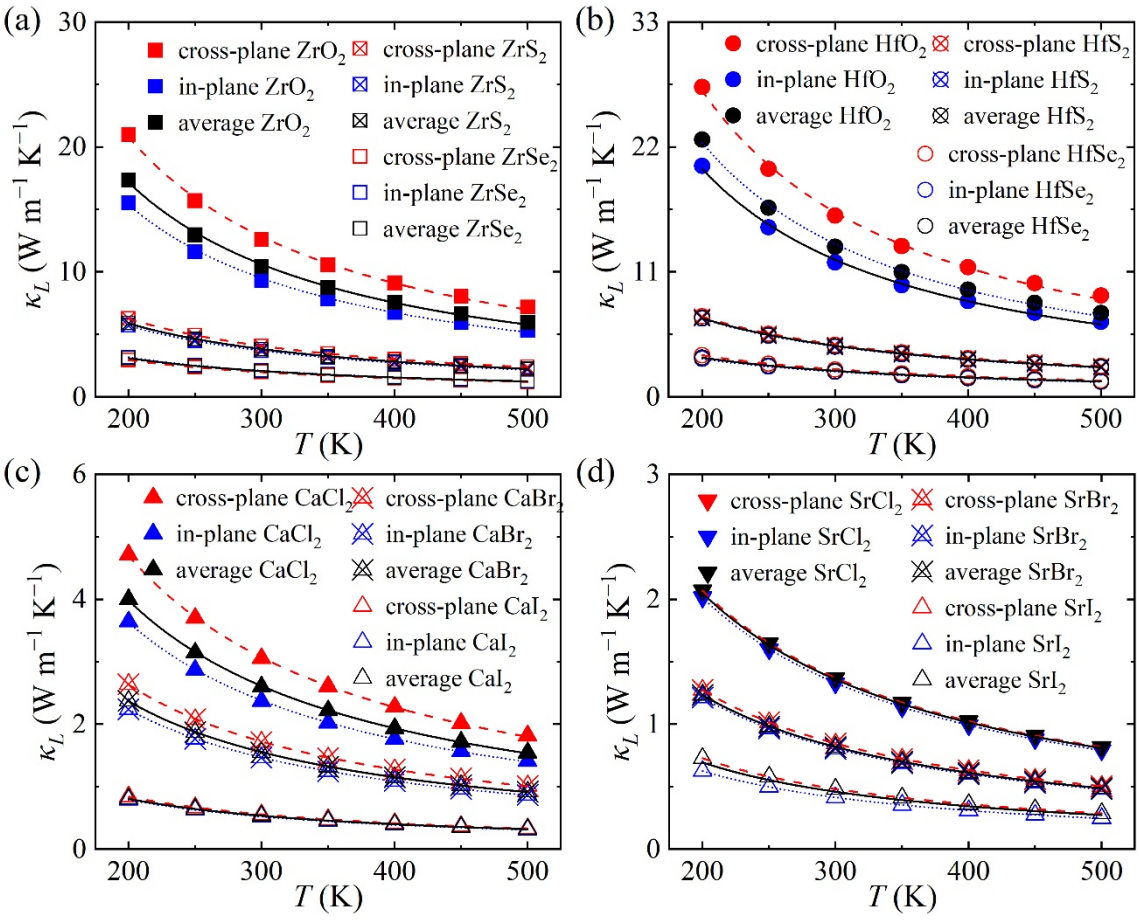

Fig. S3. The temperature-dependent in-plane (perpendicular to the direction of spontaneous polarization P_S), cross-plane (parallel to the direction of P_S) and average thermal conductivities κ_L for (a,b) group IV-VI and (c,d) group II-VII fluorite-

structure ferroelectrics.

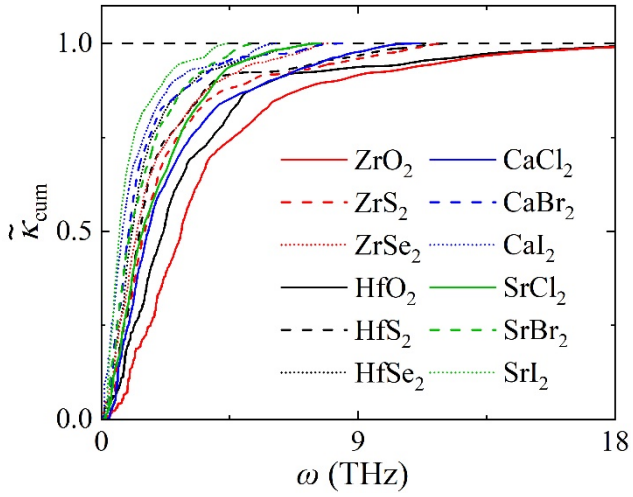

Fig. S4. Normalized cumulative thermal conductivity $\tilde{\kappa}_{cum}$ for fluorite-structure ferroelectrics.