Supporting Information

Remarkable thermoelectric performance in K_2CdPb crystal with 1D building blocks via structure particularity and bond heterogeneity

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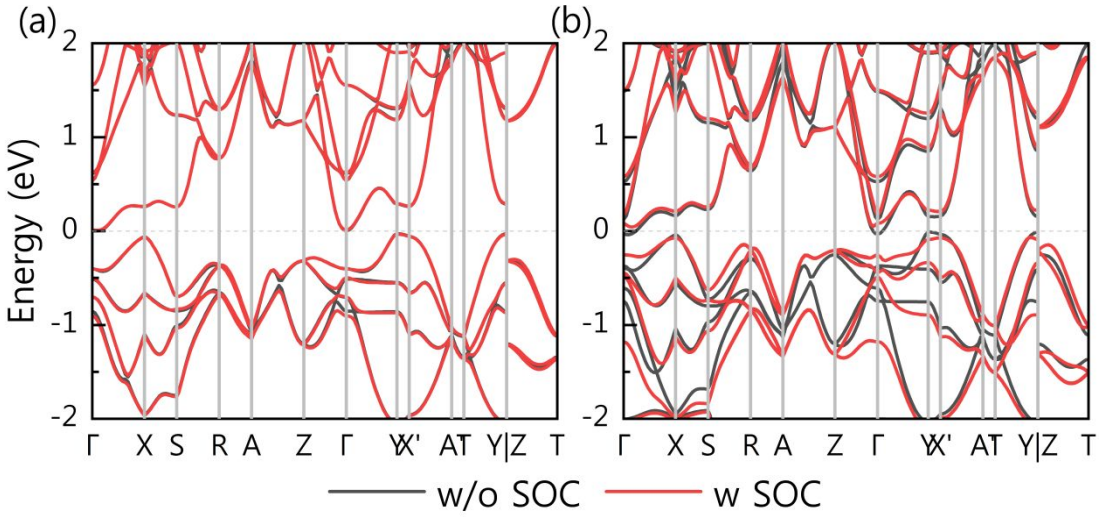

Figure S1 Comparison of band structure calculated with (red line) and without (black line) spin-orbit coupling (SOC) effect for (a) K_2CdSn and (b) K_2CdPb.

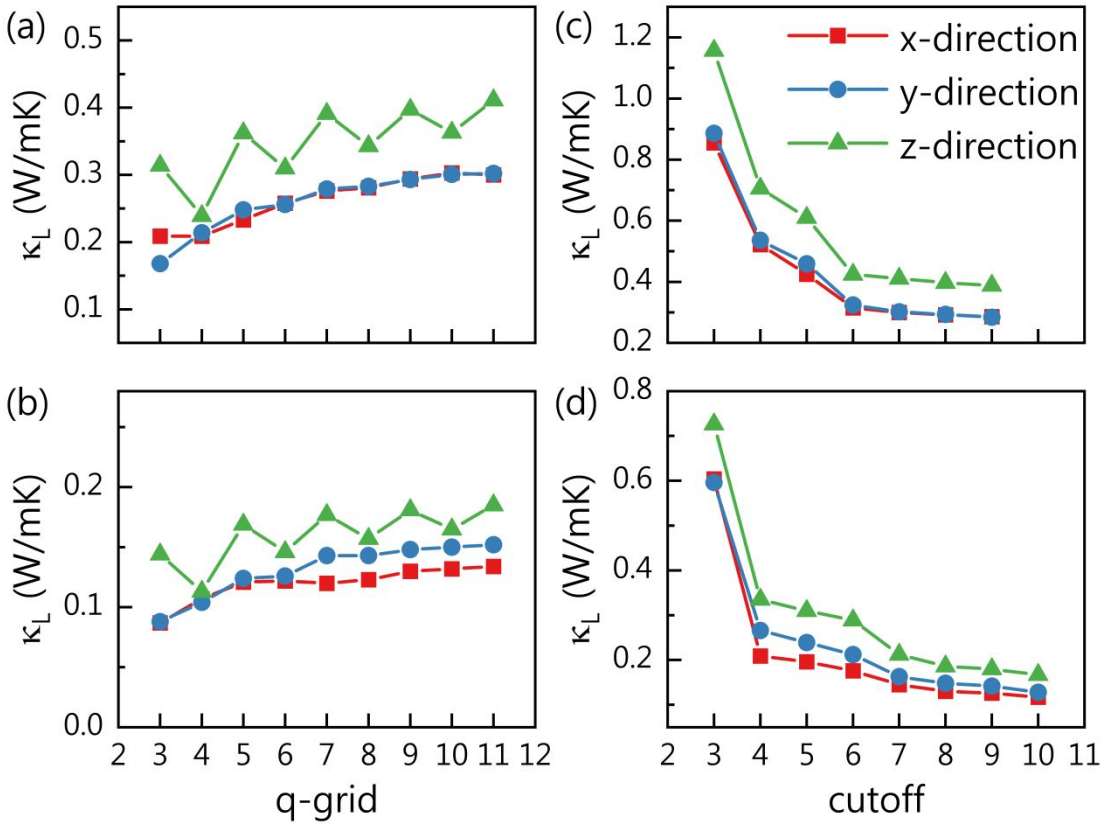

Figure S2 Convergence test of the lattice thermal conductivity (κ_L) with respect to (a) (b) q-mesh and (c) (d) interaction cutoff for K_2CdSn (upper panel) and K_2CdPb (lower panel), respectively. The red, blue and green lines indicate the κ_L along the x-, y- and z-direction, respectively.

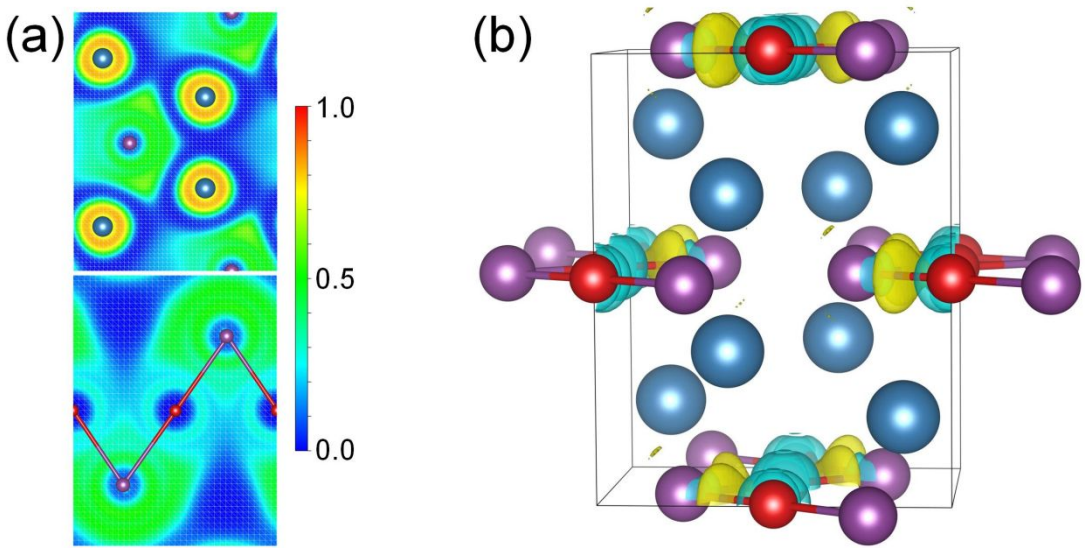

Figure S3 (a) The electron localization function (ELF) in the (100) plane (upper) and (001) plane (lower), and (b) charge density difference of K_2CdPb. The blue, red and purple balls represent K, Cd and Pb atoms, respectively. The accumulative (depleted) electrons are represented by yellow (blue) iso-surfaces.

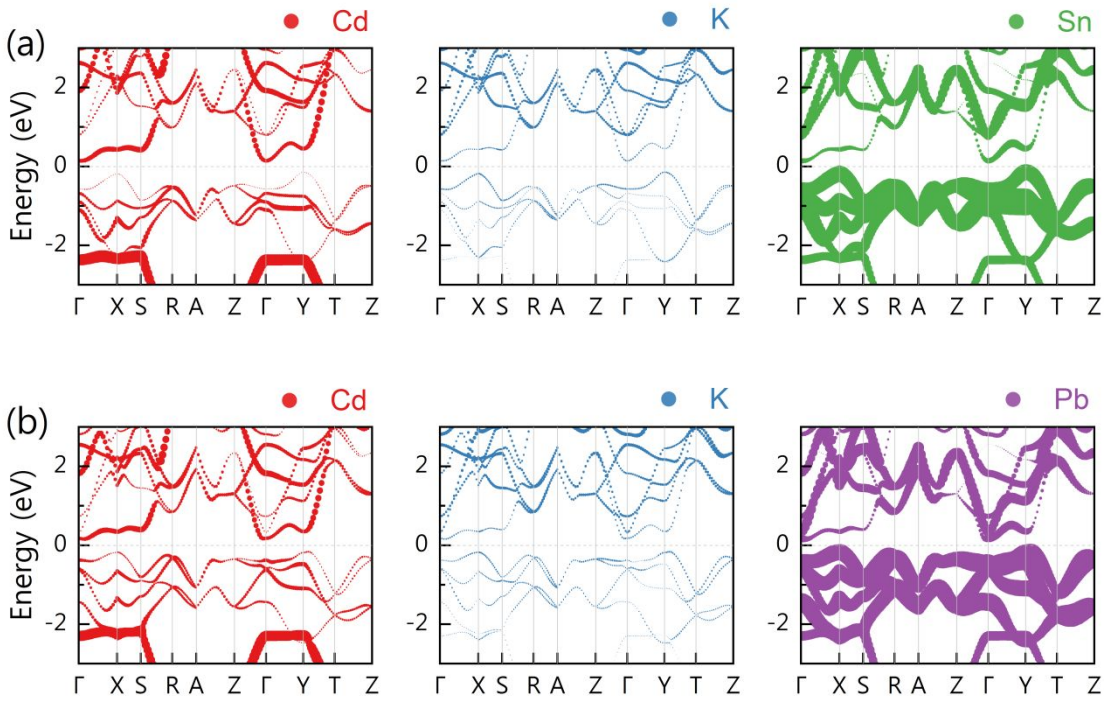

Figure S4 The decomposed band structure of (a) K_2CdSn and (b) K_2CdPb. The red, blue, green and purple circles denote the projected band structure of Cd, K, Sn and Pb element, respectively.

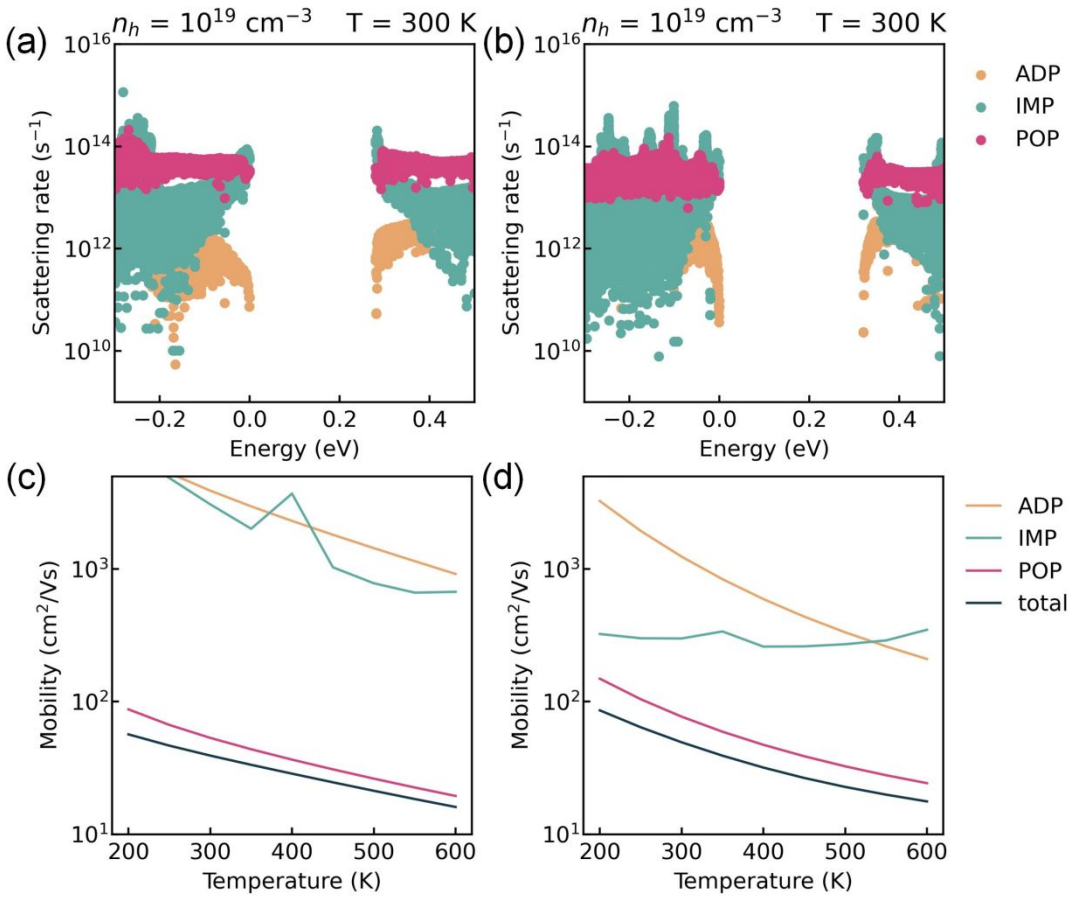

Figure S5 (a) (b) Calculated room temperature scattering rates and (c) (d) variation of mobility with temperature at the hole concentration of 10^{19} cm^3 for K_2CdSn (left panel) and K_2CdPb (right panel) limited by acoustic deformation potential (ADP, orange circle or line), ionized impurity (IMP, cyan circle or line) and polar optical phonon (POP, magenta circle or line) scattering processes. The black line indicates the mobility obtained by considering the three scattering mechanisms.

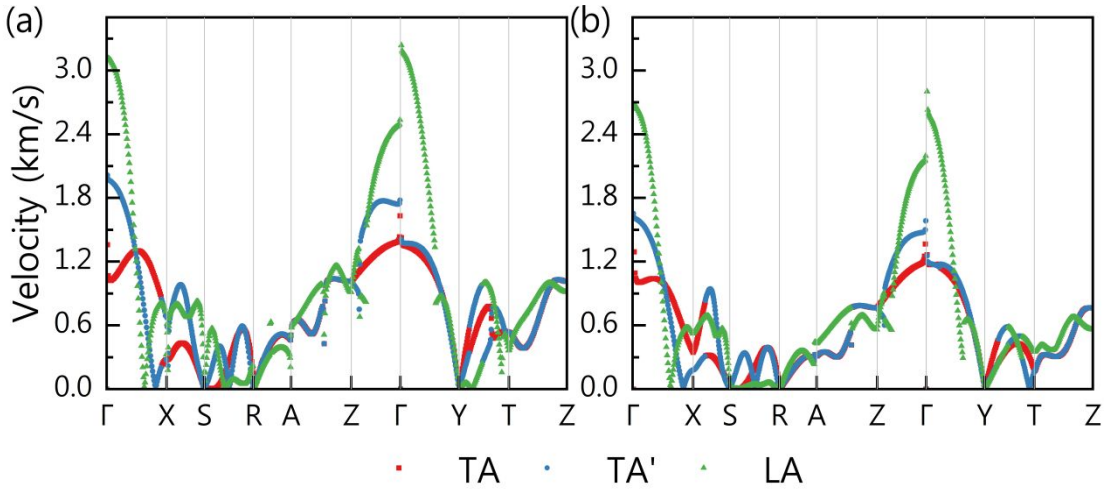

Figure S6 Phonon group velocity (transverse acoustic (TA, TA′) and longitudinal acoustic (LA)) along the high symmetry path for (a) K_2CdSn and (b) K_2CdPb. The TA, TA′ and LA are colored by red, blue and green, respectively.

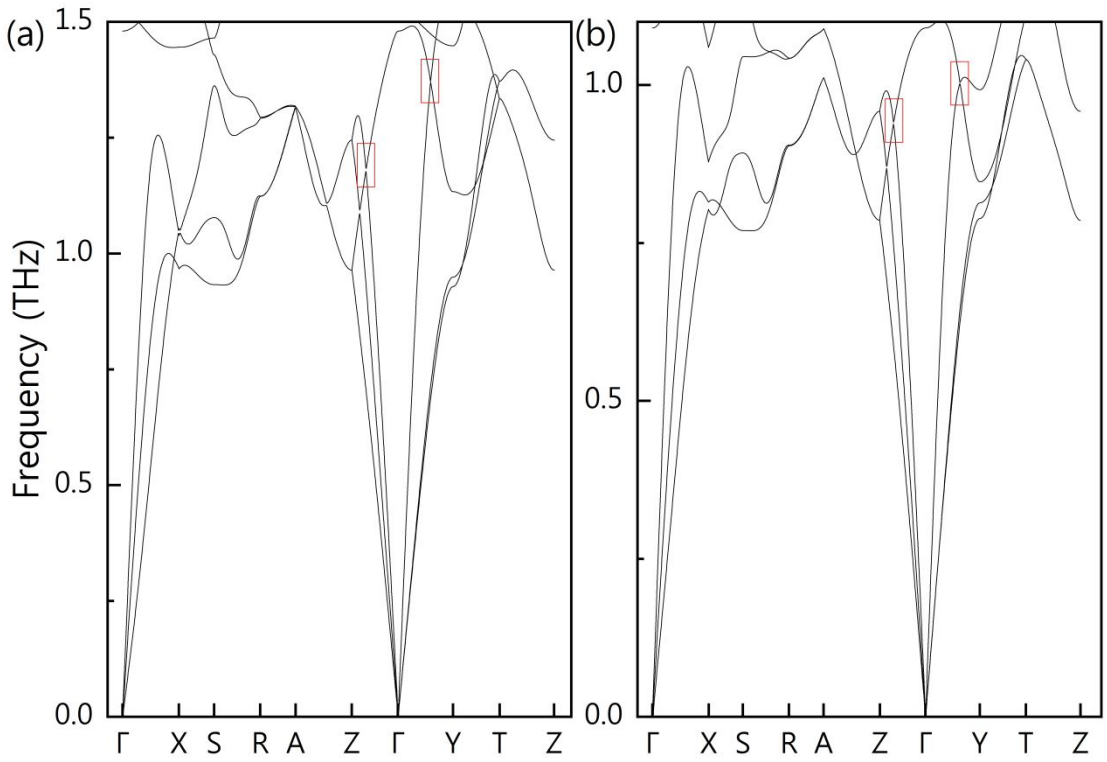

Figure S7 Enlarged phonon spectrum of (a) K_2CdSn and (b) K_2CdPb, the regions marked by red rectangle denote the avoided crossing between the acoustic and optical modes.

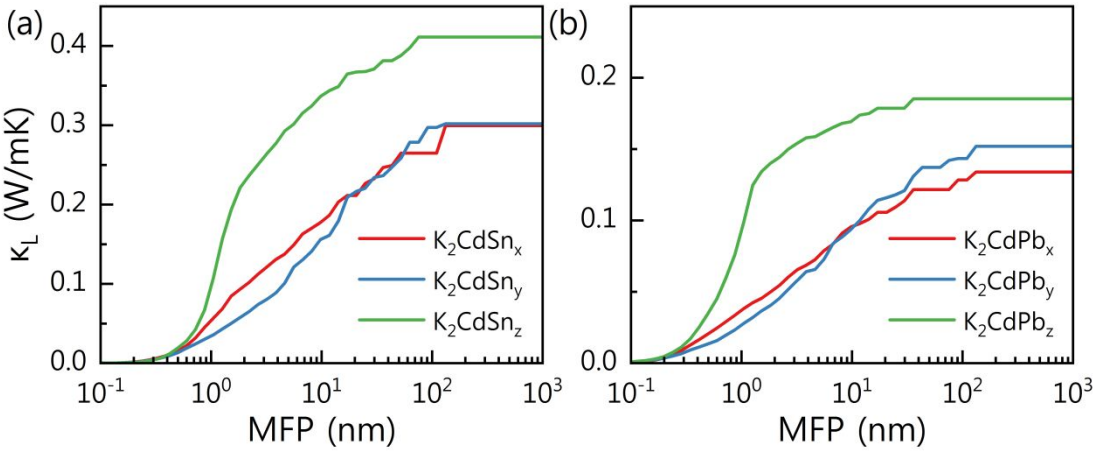

Figure S8 Accumulative κ_L with respect to phonon mean free paths (MFP) along different directions for (a) K_2CdSn and (b) K_2CdPb.

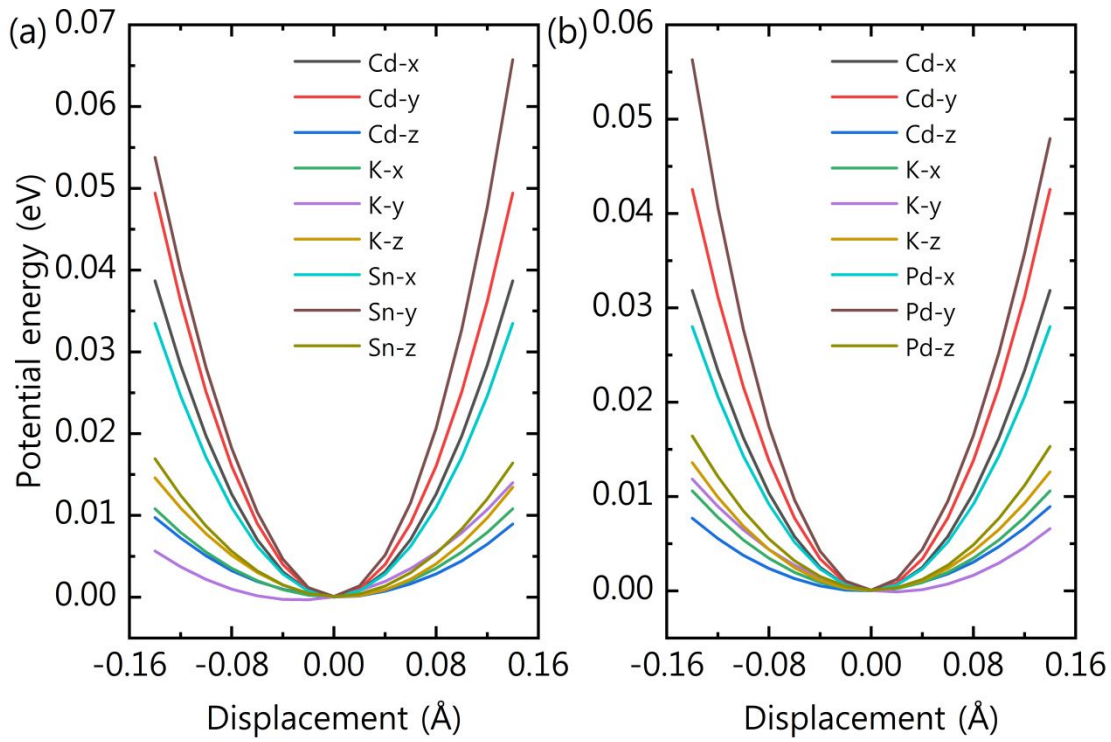

Figure S9 Potential energy of atoms with displacement along x-, y- and z-directions for (a) K_2CdSn and (b) K_2CdPb.

Table S1 The relevant parameters used to compute scattering rate. C (in GPa) is elastic tensor, ε_s and ε_∞ (in ε_0) are static and high-frequency dielectric constants, respectively. ω_{PO} (in THz) is effective polar phonon frequency.

	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	ε_s^{11}	ε_s^{22}	ε_s^{33}	ε_∞^{11}	ε_∞^{22}	ε_∞^{33}	ω_{PO}
K_2CdS	30.	31.	22.	6.	14.	6.	5.	12.	5.	20.	15.	22.	14.	12.	15.	2.8
n	7	8	3	4	7	3	9	7	1	6	9	5	6	7	9	4
K_2CdP	28.	29.	20.	6.	12.	6.	5.	11.	4.	31.	22.	28.	21.	19.	21.	2.6
b	7	3	1	2	9	0	7	6	7	5	6	3	7	6	5	6