Supporting Information

Bonding heterogeneity inducing low lattice thermal conductivity and high thermoelectric performance in 2D $CdTe_2$

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Table S1. Lattice parameters, space group (SG) and atomic position of predicted 2D CdTe and $CdTe_2$

Compound	SG	Lattice parameters			Site		Special position		
		a	b	c			x	y	z
CdTe	*P-3m1*	4.670		14.515	Cd	2d	0.3333	0.6667	0.4277
					Te	2d	0.6667	0.3333	0.3617
$CdTe_2$	*P-4$_2$1m*	10.938		15.333	Cd	2b	0.0000	0.0000	0.5000
					Te	4e	0.6611	0.1611	0.5997

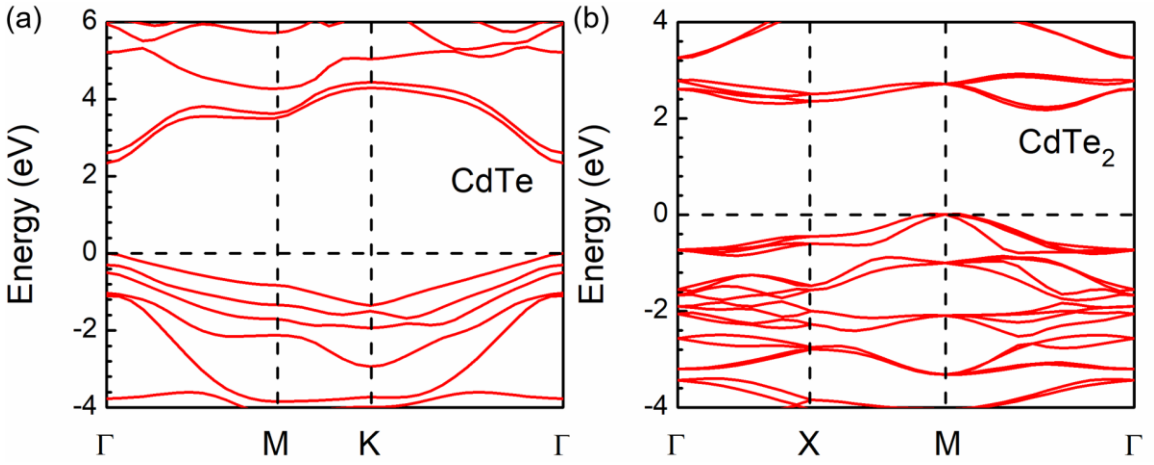

Figure S1. Band structures for CdTe (a) and $CdTe_2$ (b) with HSE06+SOC correction.

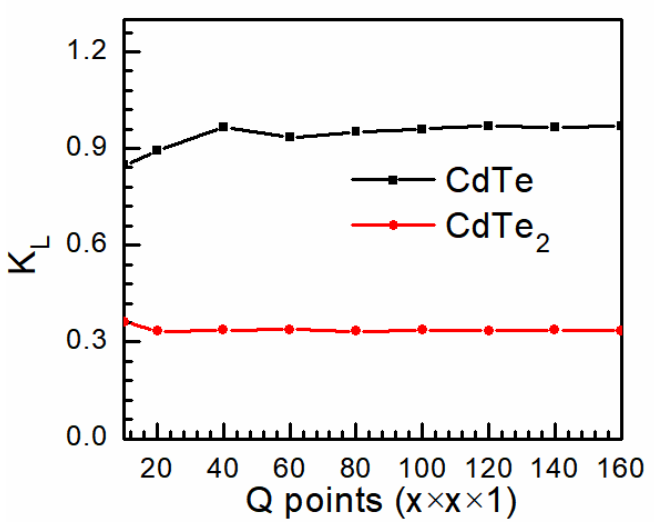

Figure S2. K_L at 300 K of CdTe and $CdTe_2$ as a function of Q points.

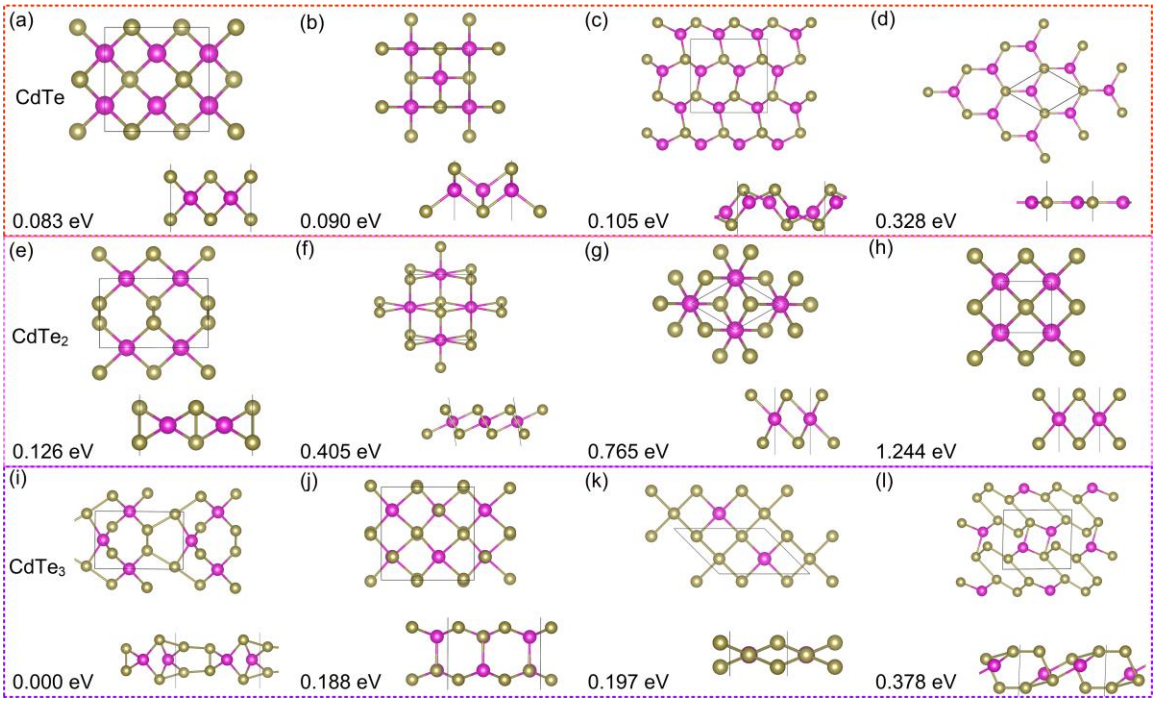

Figure S3. Top and side views of metastable 2D CdTe (a-d), $CdTe_2$ (e-h) and $CdTe_3$ (i-l). The left corner is calculated energy (per formula) relative to the most stable 2D CdTe, $CdTe_2$ and $CdTe_3$, respectively.

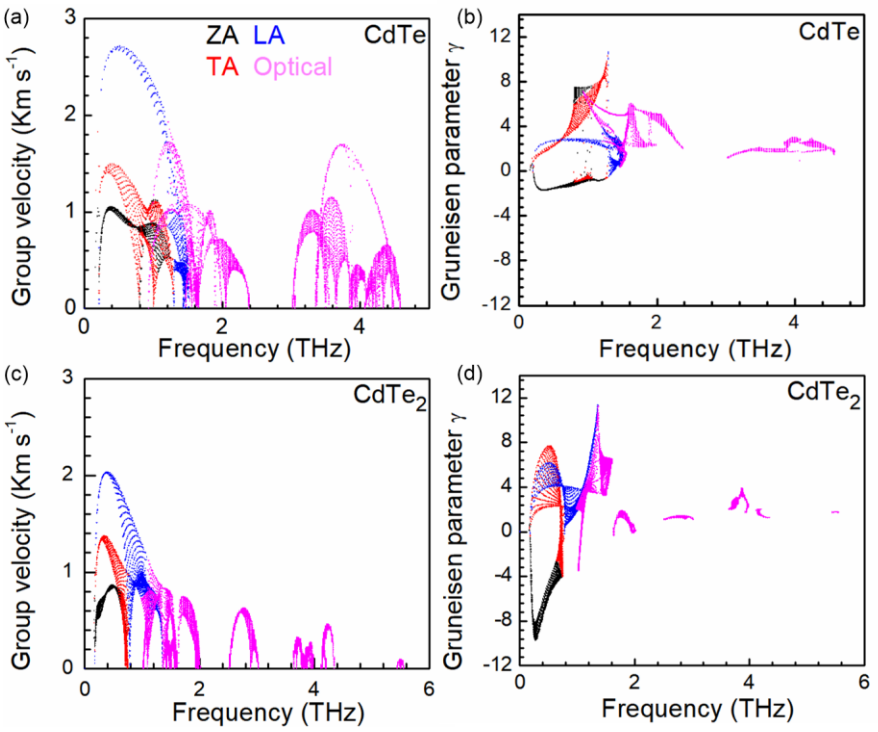

Figure S4. Group velocity at 300 K for CdTe (a) and $CdTe_2$ (c), and mode-Gruneisen parameter for CdTe (b) and $CdTe_2$ (d).

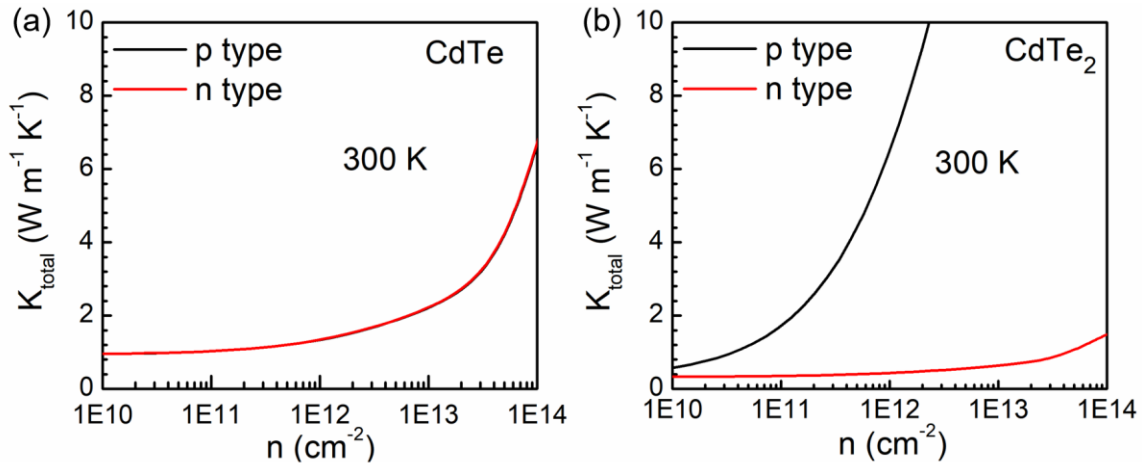

Figure S5. Total thermal conductivity ($\kappa_L+\kappa_e$) for CdTe (a) and $CdTe_2$ (b) at 300 K.