Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Pressure induced phase transitions of bulk $CsGeCl_3$ and ultrafast laser pulses induced excited-state properties of $CsGeCl_3$ quantum dots

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Table S1. Lattice parameters (a, b, c) and reduced atomic coordinates (*x*, *y*, *z*) of $CsGeCl_3$ for the *R3m* (0 GPa), *Cm* (0 GPa), *Pm*$\bar{3}$*m* (9 GPa), ppPv-*Pnma* (40 GPa), and *I4mm* (100 GPa), respectively.

			Coordinates		
	Atoms	Wyck.	*x*	*y*	*z*
R3m			a=7.4625Å	b=7.4625Å	c=9.1906Å
(0 GPa)			α=90°	β=90°	γ=120°
	Cs	3a	0.00000	0.00000	0.82449
	Ge	3a	0.66667	0.33333	0.64539
	Cl	9b	0.49106	0.98211	0.83505
Cm			a=7.4907Å	b=7.4619Å	c=5.2887Å
(0 GPa)			α=90°	β=89.6633°	γ=90°
	Cl	4b	0.74074	0.23662	0.98886
	Cl	2a	0.00415	0.50000	0.46214
	Cs	2a	0.00578	-0.00000	0.49057
	Ge	2a	0.51819	-0.00000	0.00354
Pm$\bar{3}$*m*			a=4.8976Å	b=4.8976Å	c=4.8976Å
(9 GPa)			α=90°	β=90°	γ=90°
	Cs	1a	0.00000	0.00000	0.00000
	Ge	1b	0.50000	0.50000	0.50000
	Cl	3c	-0.00000	0.50000	0.50000
ppPv-*Pnma*			a=7.8253Å	b=3.1454Å	c=13.7519Å
(40 GPa)			α=90°	β=90°	γ=90°
	Cs	4c	0.54848	0.25000	0.84780
	Ge	4c	0.42136	0.25000	0.43675
	Cl	4c	0.29301	0.25000	-0.00332
	Cl	4c	0.91392	0.25000	0.84718
	Cl	4c	0.76088	0.25000	0.19868
I4mm			a=3.0417Å	b=3.0417Å	c=14.2074Å
(100 GPa)			α=90°	β=90°	γ=90°
	Cs	2a	0.00000	-0.00000	0.23278
	Cl	2a	0.00000	-0.00000	0.61446
	Cl	2a	0.00000	-0.00000	0.44001
	Ge	2a	-0.50000	0.50000	0.51642
	Cl	2a	-0.50000	0.50000	0.34796

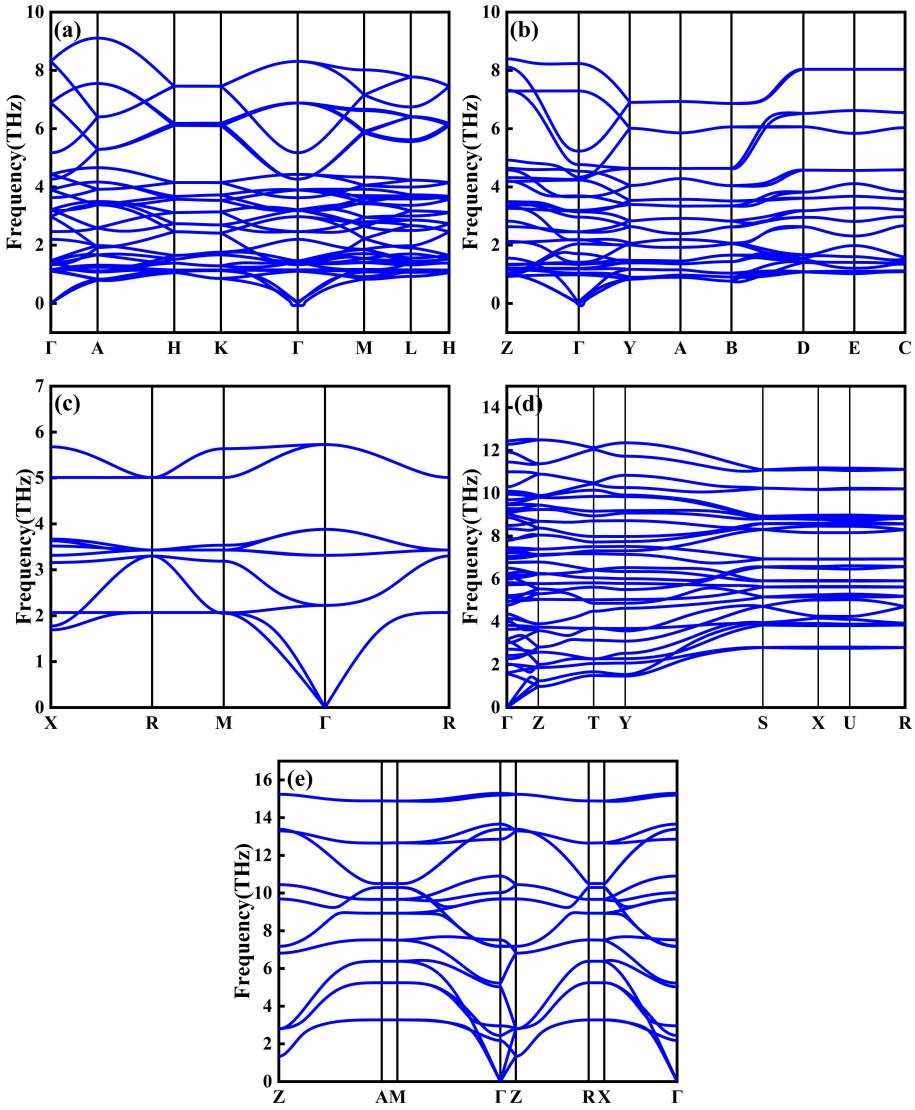

Fig. S1. Calculated phonon dispersions for (a) *R3m* at 0 GPa, (b) *Cm* at 0 GPa, (c) *Pm*$\bar{3}$*m* at 9 GPa, (d) ppPv-*Pnma* at 40 GPa, and (e) *I4mm* at 100 GPa, respectively.

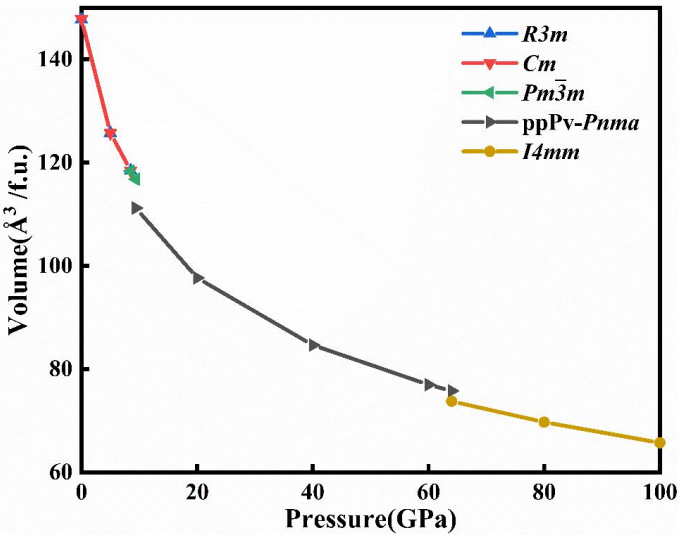

Fig. S2. The volume of different structures for $CsGeCl_3$ as a function of pressure.

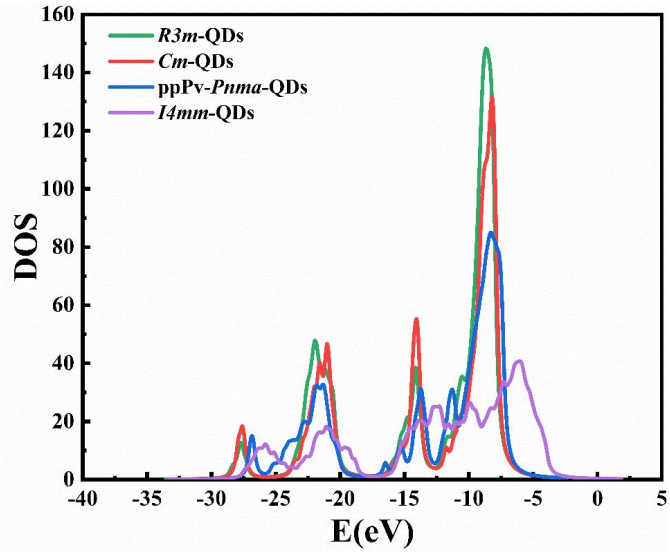

Fig. S3. The density of states (DOS) obtained from the ground-state information for *R3m*-QDs, *Cm*-QDs, ppPv-*Pnma*-QDs, and *I4mm*-QDs, respectively.

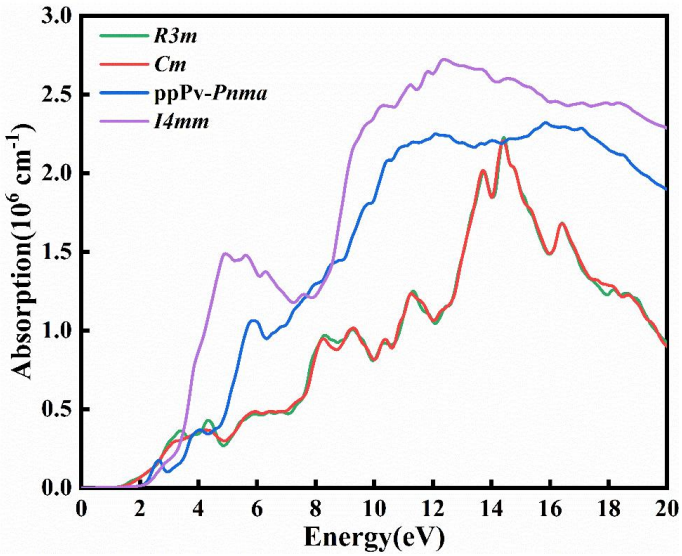

Fig. S4. The absorption spectra of bulk structures $CsGeCl_3$ for *R3m* (0 GPa), *Cm* (0 GPa), ppPv-*Pnma* (40 GPa), and *I4mm* (100 GPa), respectively.

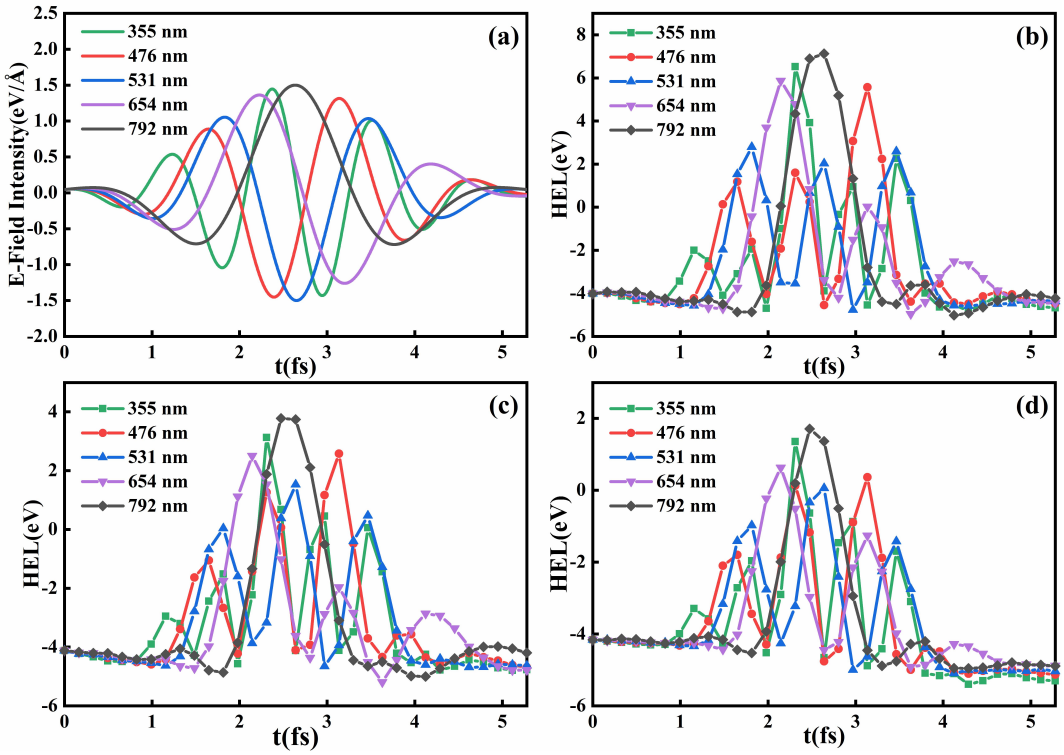

Fig. S5. (a) The laser oscillograph, (b)-(d) the HEL in *R3m*-QDs, *Cm*-QDs, and ppPv-*Pnma*-QDs with ultrafast lasers for the intensity of 1.5 eV/Å and the different wavelengths of 355 nm, 476 nm, 531 nm, 654 nm, and 792 nm are selected, respectively.