Supplementary materials of "Reverse charge transfer and decomposition in Ca-Te compounds under high pressure"

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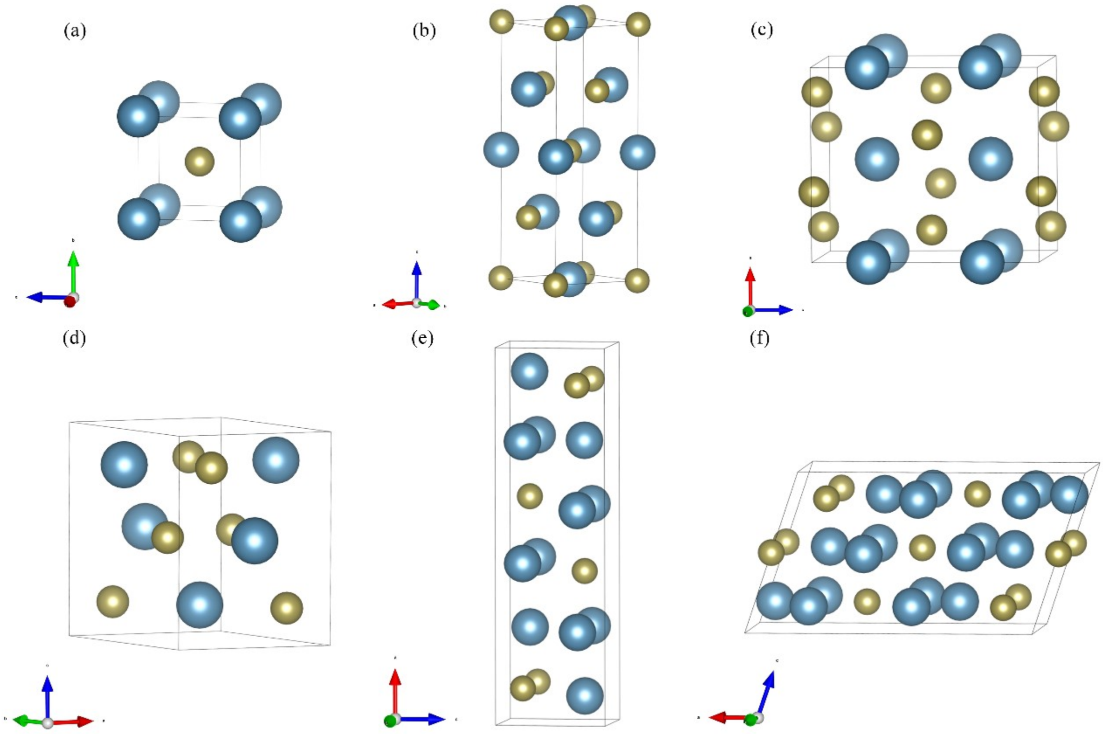


Fogure S1. Predicted crystal structures. (a) *Pm*-3*m,* CaTe. (b) *I*41/*amd*, CaTe. (c) *I*4/*mcm*, CaTe. (d) *P*6422, $CaTe_2$ (e) *Cmcm*, Ca_2Te. (f) *C*2/*m*, Ca_2Te.

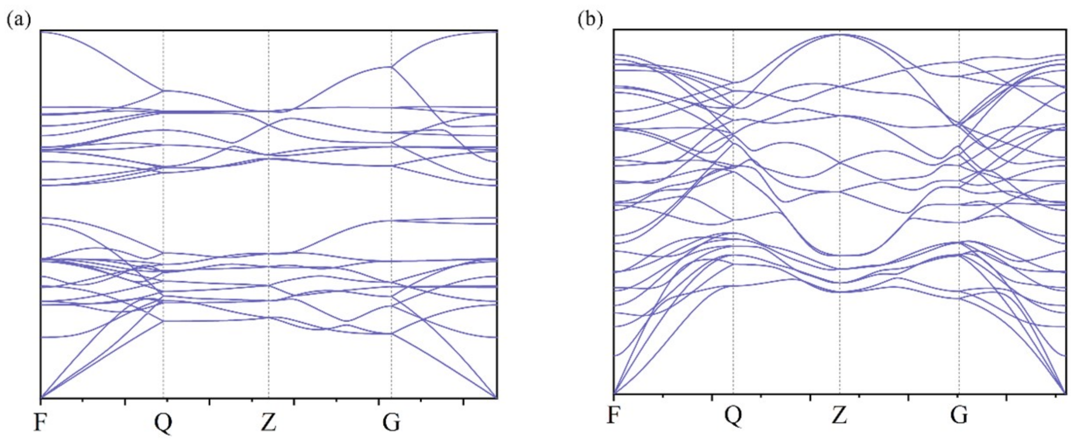


Figure S2. Calculated phonon dispersion curves. (a) *I*4/*mcm*, $CaTe_2$. (b) *Cmcm*, Ca_2Te.

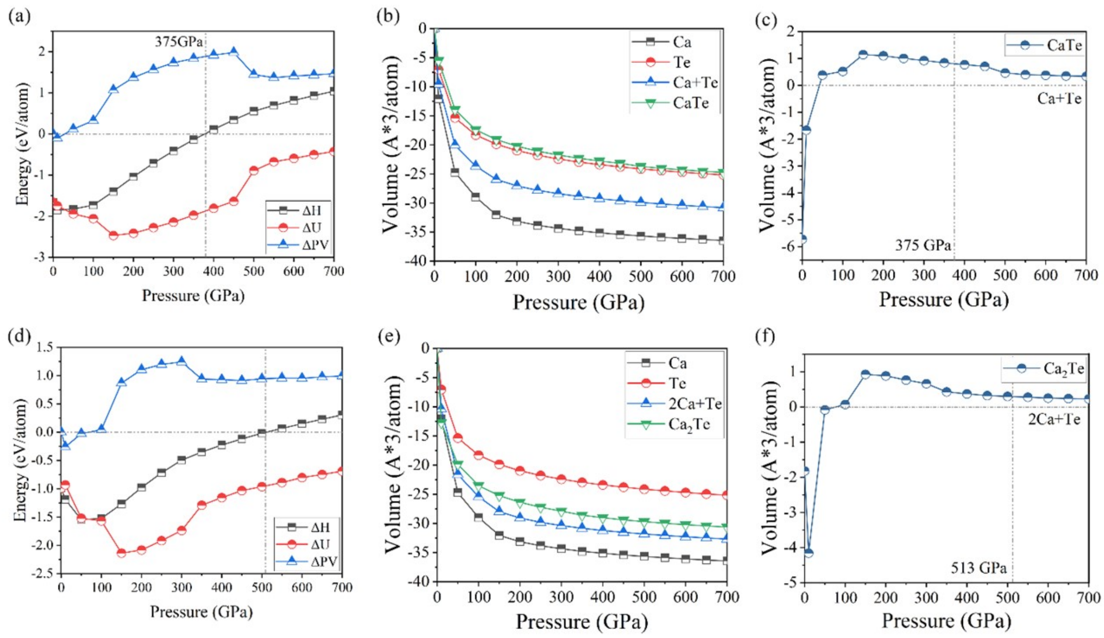


Figure S3. Electronic properties under different pressure. (a) △H,△U, and P△V versus pressure for CaTe. (b) The volume of Ca elemental, Te elemental, Ca and Te mixture, and CaTe compound as a function of pressure. (c) The volume differences between the compound (CaTe) and Ca + Te. (d) △H,△U, and P△V versus pressure for Ca2Te. (e) The volume of Ca elemental, Te elemental, Ca and Te mixture and Ca2Te compound as a function of pressure. (f) The volume differences between the compound (Ca2Te) and 2Ca + Te.

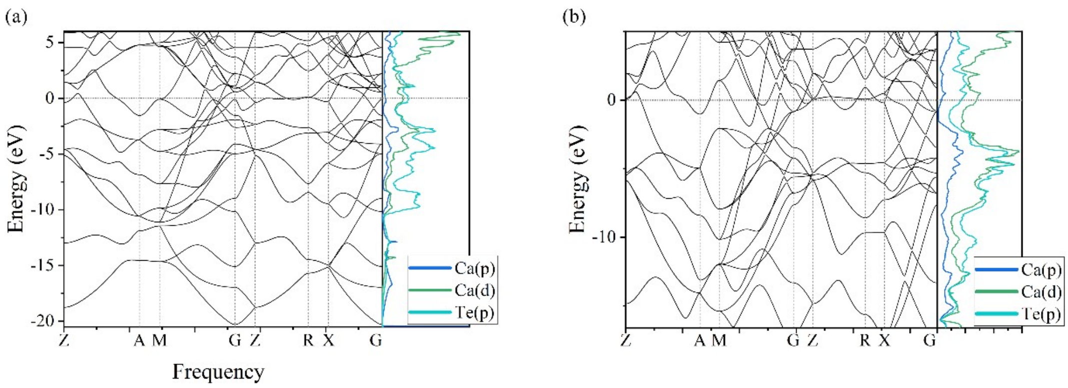


Figure S4. (a) Band and PDOS of $CaTe_2$ as the pressure of 200 GPa. (b) Band and PDOS of $CaTe_2$ as the pressure of 600 GPa.

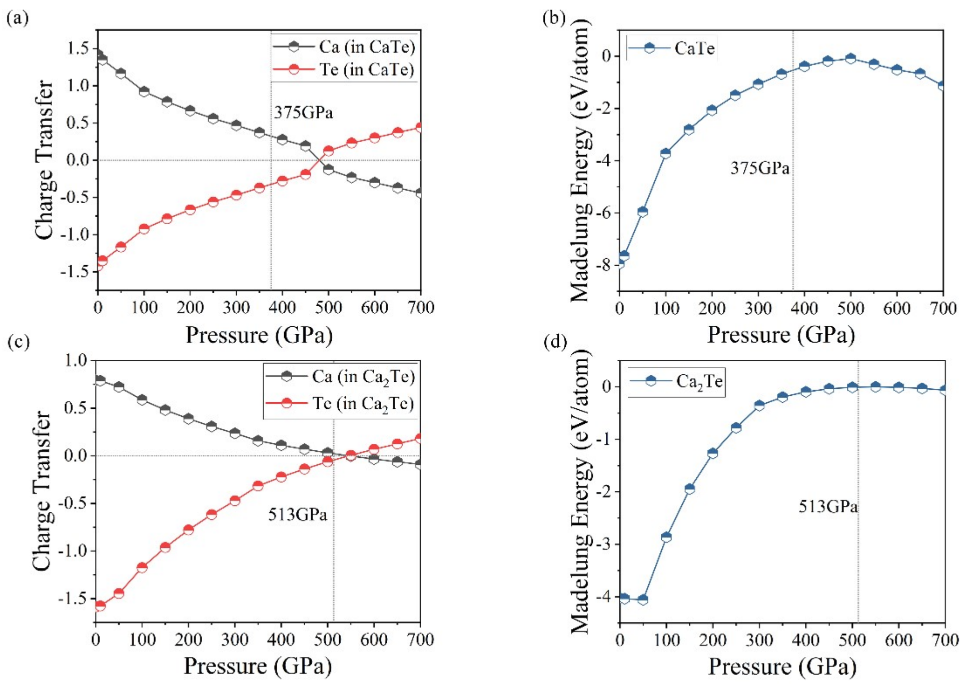


Figure S5. (a) The Bader charge of Ca and Te in CaTe. (b) The Madelung energy of CaTe. (c) The Bader charge of Ca and Te in Ca2Te. (d) The Madelung energy of Ca_2Te.

Table S1.

Elastic constants (in GPa) of Ca_2Te and criteria for elastic stability:

$$C_{ij}(Cmcm) = \begin{pmatrix} 83.746 & 17.642 & 16.844 & & & \\ & 99.950 & 42.535 & & & \\ & & 73.965 & & & \\ & & & 13.604 & & \\ & & & & 60.147 & \\ & & & & & 37.177 \end{pmatrix}$$

1. 1. $C_{ii} > 0$
2. $C_{11}C_{22} > C_{12}^2$
3. $C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} - C_{11}C_{23}^2 - C_{22}C_{23}^2 - C_{33}C_{23}^2 > 0$

$$C_{ij}(C2/m) = \begin{pmatrix} 344.504 & 160.374 & 169.161 & & & \\ & 327.674 & 150.465 & & & \\ & & 485.416 & & & \\ & & & 212.813 & & \\ & & & & 107.916 & \\ & & & & & 108.527 \end{pmatrix}$$

1. $C_{ii} > 0$
2. $D_1 = C_{11}C_{22} - C_{12}^2 > 0$
3. $D_2 = C_{11}C_{33} - C_{13}^2 > 0$
4. $D_3 = C_{22}C_{33} - C_{23}^2 > 0$
5. $D_1D_2 - D_3^2 > 0$

Elastic constants (in GPa) of CaTe and criteria for elastic stability:

$$C_{ij}(I4_1amd) = \begin{pmatrix} 345.516 & 321.343 & 153.970 & & & -0.137 \\ & 345.907 & 154.163 & & & -0.190 \\ & & 422.047 & & & \\ & & & 285.495 & & \\ & & & & 149.229 & \\ & & & & & 148.102 \end{pmatrix}$$

1. $C_{ii} > 0$
2. $C_{11} > |C_{12}|$
3. $2C_{12}^2 < C_{33}(C_{11} + C_{12})$
4. $2C_{16}^2 < C_{66}(C_{11} - C_{12})$

Elastic constants (in GPa) of $CaTe_2$ and criteria for elastic stability:

$$C_{ij}(I4/mcm) = \begin{pmatrix} 117.814 & 68.209 & 37.501 & & & -0.079 \\ & 117.692 & 37.422 & & & -0.098 \\ & & 86.575 & & & \\ & & & 62.748 & & \\ & & & & 41.637 & \\ & & & & & 41.645 \end{pmatrix}$$

1. $C_{ii} > 0$
2. $C_{11} > |C_{12}|$
3. $2C_{12}^2 < C_{33}(C_{11} + C_{12})$
4. $2C_{16}^2 < C_{66}(C_{11} - C_{12})$

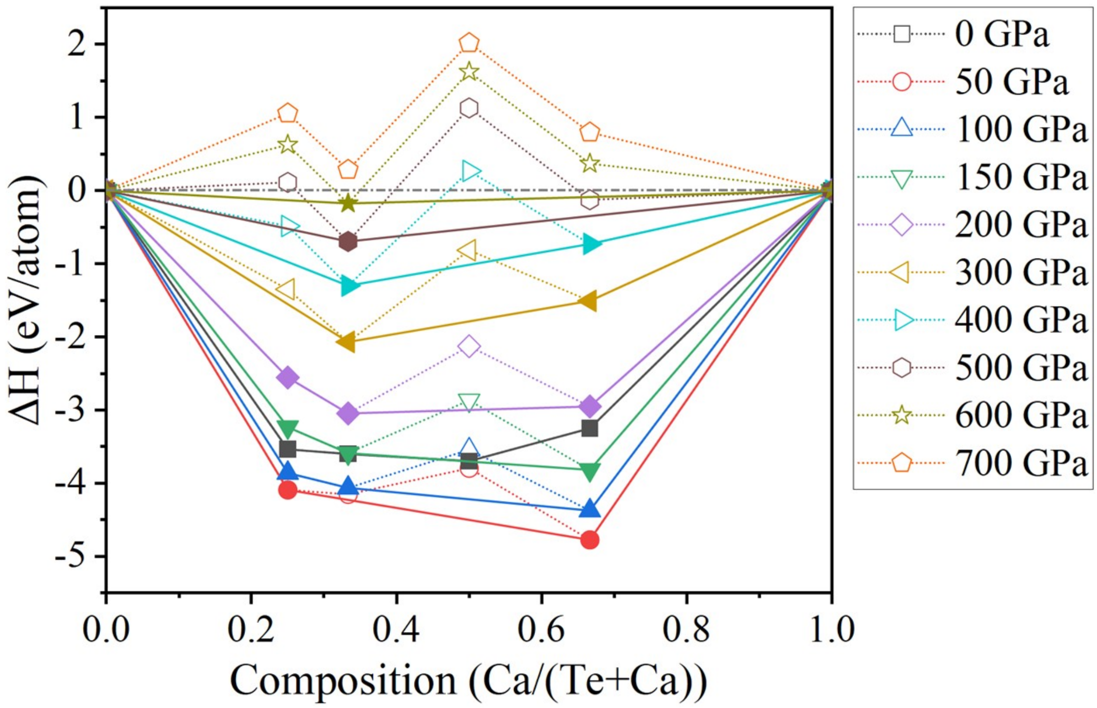
$$C_{ij}(P6_422) = \begin{pmatrix} 279.084 & 114.123 & 97.945 & & & \\ & 277.267 & 97.817 & & & \\ & & 364.074 & & & \\ & & & 81.519 & & \\ & & & & 44.632 & \\ & & & & & 44.673 \end{pmatrix}$$

1. $C_{ii} > 0$
2. $C_{11} > |C_{12}|$
3. $2C_{12}^2 < C_{33}(C_{11} + C_{12})$

$$C_{ij}(I4mmm) = \begin{pmatrix} 317.706 & 288.359 & 203.842 & & & \\ & 317.622 & 203.818 & & & \\ & & 435.733 & & & \\ & & & 298.109 & & \\ & & & & 200.860 & \\ & & & & & 199.287 \end{pmatrix}$$

1. $C_{ii} > 0$
2. $C_{11} > |C_{12}|$
3. $2C_{12}^2 < C_{33}(C_{11} + C_{12})$

(a)



(b)

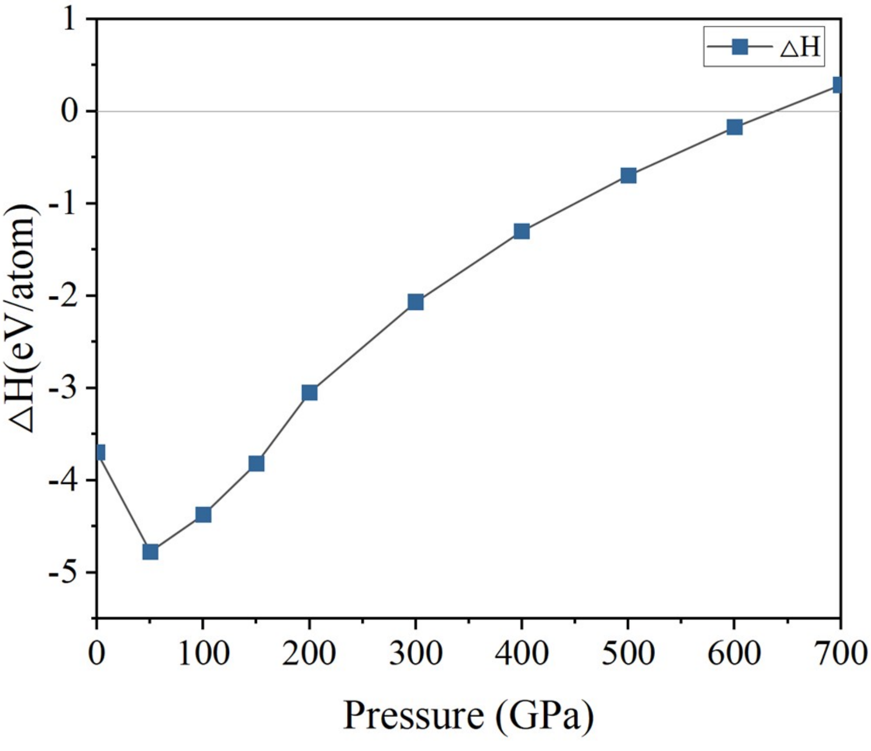


Figure S6. (a) Convex hull graph obtained by MetaGGA method. (b)The enthalpy of the most stable compound in the system as a function of pressure.

(a)

100 GPa		**Bader Charge**	**Mulliken Charge**	**Loewdin Charge**
Charge	**Ca (e)**	-0.8579	1.1588	1.3075
	Te (e)	-0.4022	-0.5813	-0.6538
Madelung energy (eV/atom)		-1.5468	-2.8342	-3.6008

(b)

600 GPa		**Bader Charge**	**Mulliken Charge**	**Loewdin Charge**
Charge	**Ca (e)**	-0.2443	0.7463	1.1754
	Te (e)	-0.1222	-0.3706	-0.5877
Madelung energy (eV/atom)		-0.1524	-1.3970	-3.4550

Table S2. (a) Charge transfer and Madelung energy calculated using three different methods under a pressure of 100 GPa, based on the hybrid functional HSE06. (b) Charge transfer and Madelung energy calculated using three different methods under a pressure of 600 GPa, based on the hybrid functional HSE06.