Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Materials for

Superconductivity in Ca_3H_2 electride at moderate pressure

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Table S1. The atomic Wyckoff positions for *P63/mmc* Ca_3H_2 at different pressures

Pressure (GPa)	Atom	Site	x	y	z
0	Ca1	2c	0.67	0.33	0.75
	Ca2	4f	0.33	0.67	0.91
	H1	4f	0.67	0.33	0.63
6.8	Ca1	2c	0.67	0.33	0.75
	Ca2	4f	0.33	0.67	0.91
	H1	4f	0.67	0.33	0.63
10	Ca1	2c	0.67	0.33	0.75
	Ca2	4f	0.33	0.67	0.91
	H1	4f	0.67	0.33	0.63
14	Ca1	2c	0.67	0.33	0.75
	Ca2	4f	0.33	0.67	0.91
	H1	4f	0.67	0.33	0.62
19.5	Ca1	2c	0.67	0.33	0.75
	Ca2	4f	0.33	0.67	0.92
	H1	4f	0.67	0.33	0.62

Table S2. T_c and dimension of reported electrides at selected pressures

Compounds	Dimension	Pressures (GPa)	T_c (K)	Reference
I-43d C12A7:e^-	0D	ambient condition	0.4	[1]
Cmcm Al_5Si	0D	15	0.15	[2]
Pnma Ca_2S	0D	50	0.26	[3]
C2/m Li_9Te	0D	50	4.01	[4]
C2/m $Li_{10}Se$	0D	50	16	[5]
P2$_1$/m Ca_3S	0D	60	7.04	[3]
R-3m Li_6C	0D	80	10	[6]
C2/m $Li_{10}Te$	0D	100	4	[4]
I4/mmm YXe_2	0D	100	0.3	[7]
Pbam YXe	0D	150	3.9	[7]
I4/mcm Y_3Xe	0D	150	6.5	[7]
C2/m Li_6Al	0D	150	29	[8]
P6/mmm $AsLi_7$	0D	150	38.4	[9]
Fm-3*m* Li_8Au	0D	250	73.1	[10]
Immm Li_5S	0D	500	8.6	[11]
P63/mcm Zr_5Sb_3	1D	ambient condition	2.3	[12]
P63/mcm Nb_5Ir_3	1D	ambient condition	9.4	[13]
P63/mmc Y_3Si	1D	50	14.49	[14]
P63/mmc Ca_3Si	1D	100	17.6	[15]
R-3m Y_2C	2D	ambient condition	0.9	[16]
R-3m Ba_2N	2D	ambient condition	3.4	[17]
P63/mmc Ca_3H_2	2D	19.5	8.4	This work
P6/mmm Li_5Si	2D	100	7.2	[18]
P-1 $Li_{11}P_2$	2D	200	4.63	[19]
C2/c Li_5P	2D	200	2.61	[19]
C2/c Li_8P	2D	200	7.15	[19]
P6/mmm Li_5C	2D	210	48.3	[20]
C2/c Li_6P	2D	270	39.3	[19]
C2/m $Li_{15}P_2$	2D	300	18.5	[19]

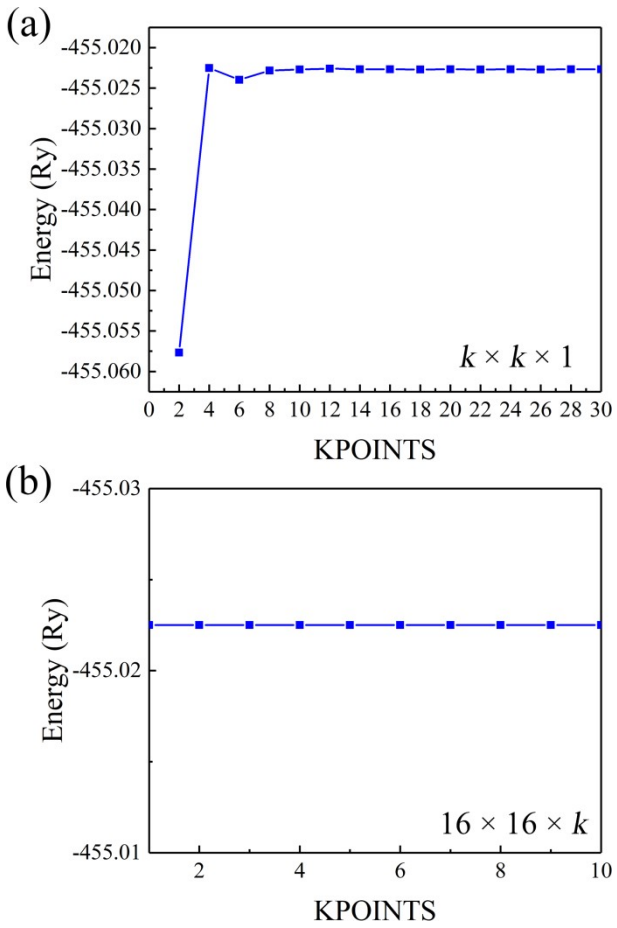

Fig. S1. The *k*-point test results for (a) c and (b) a/b directions.

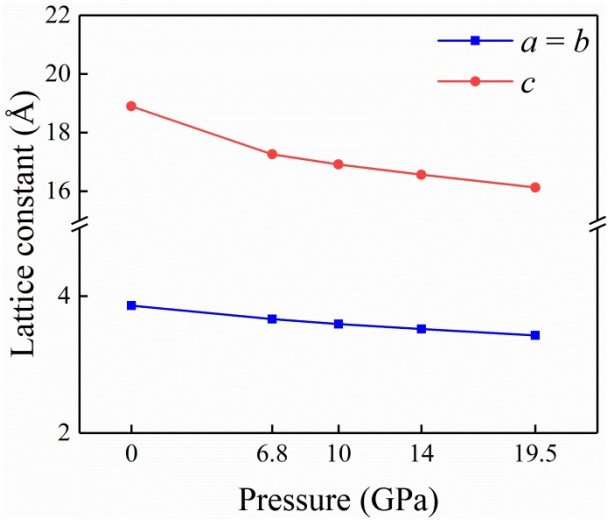

Fig. S2. The lattice constants of Ca_3H_2 at different pressures.

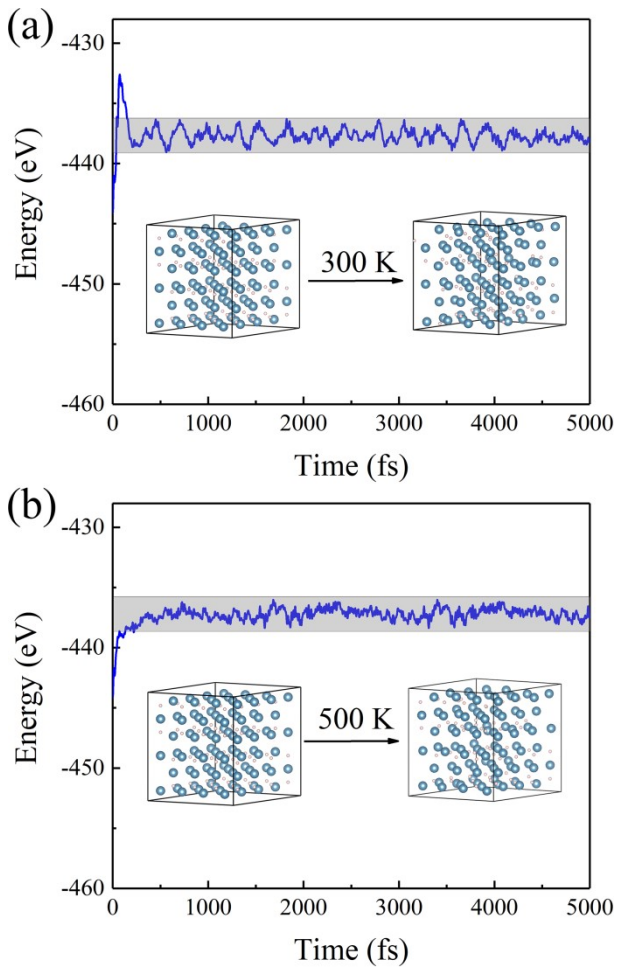

Fig. S3. Free energy evolution for Ca_3H_2 at (a) 300 K and (b) 500 K in ab initio molecules dynamic simulations under ambient condition.

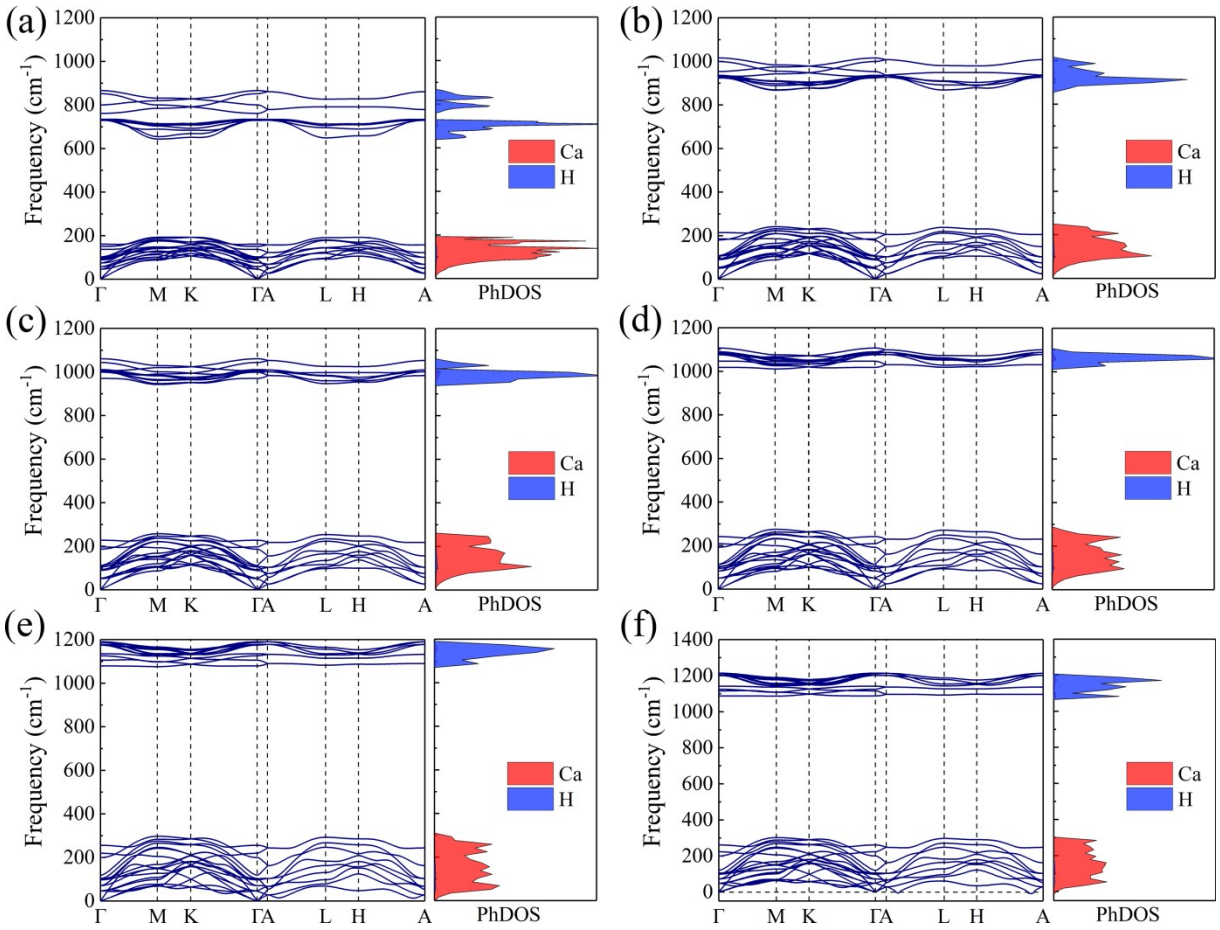

Fig. S4. Phonon dispersions and the phonon DOS for Ca_3H_2 (a) under ambient condition and at (b) 6.8 GPa, (c) 10 GPa, (d) 14 GPa, (e) 19.5 GPa, and (f) 20 GPa, respectively.

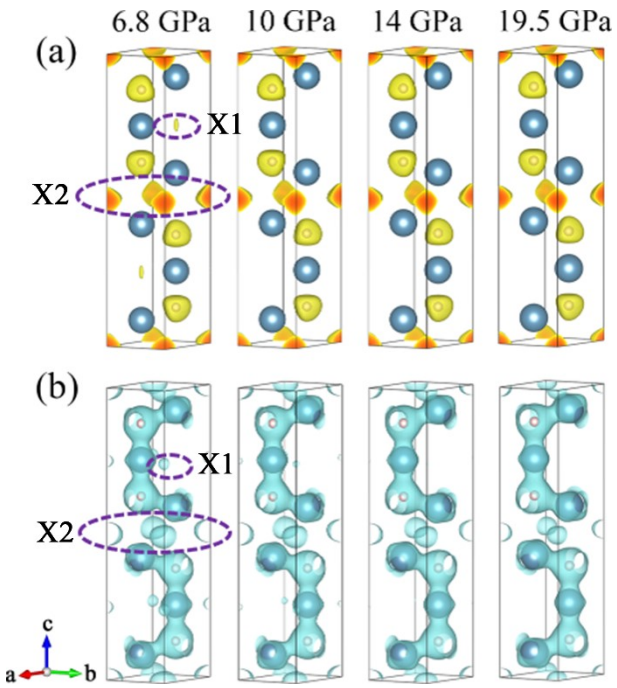

Fig. S5. (a) The ELF with an isosurface value of 0.75 and (b) ESDP with an isosurface value of -0.1 V for Ca_3H_2 at different pressures. X1, and X2 denote the different anionic electrons.

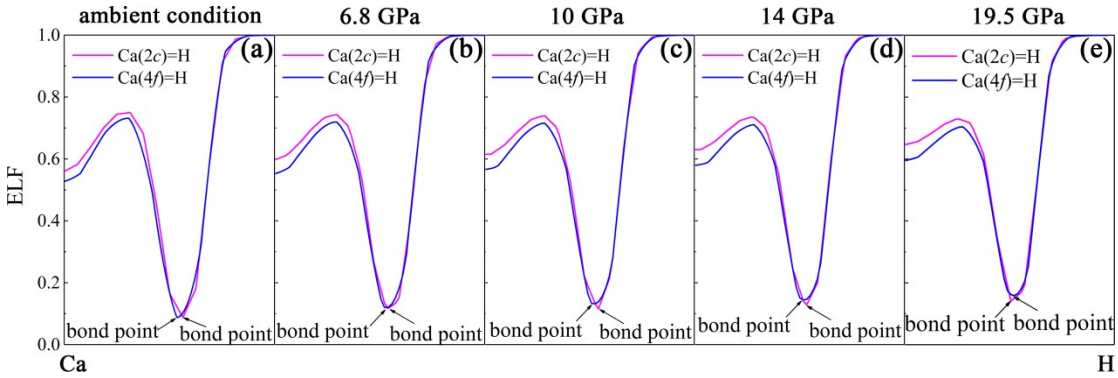

Fig. S6. The ELF 2D line profiles and bond points of the Ca–H bonds in Ca_3H_2 under different pressures.

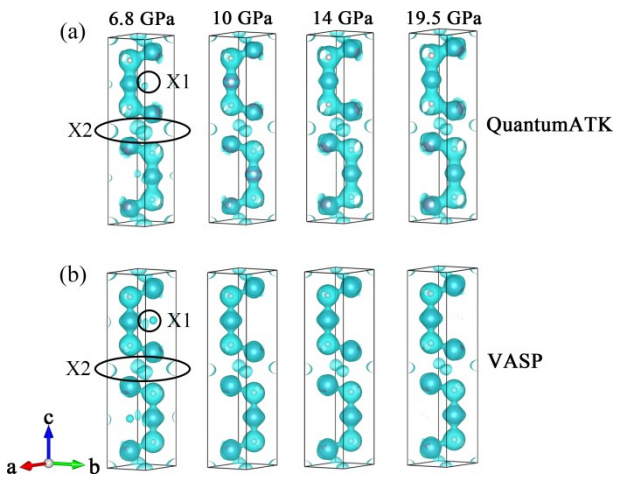

Fig. S7. The ESDP obtained separately from (a) QuantumATK and (b) (added as Fig. S4 in revised manuscript) VASP calculations.

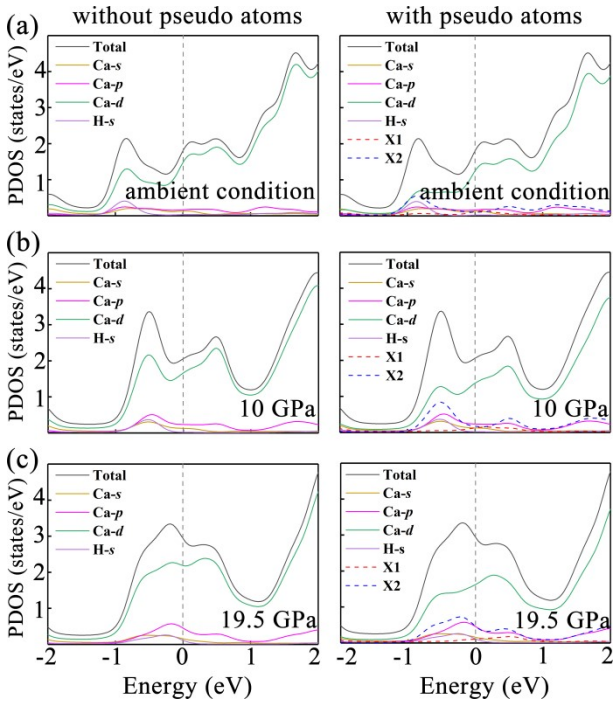

Fig. S8**.** The DOS with and without pseudo atoms under selected pressures.

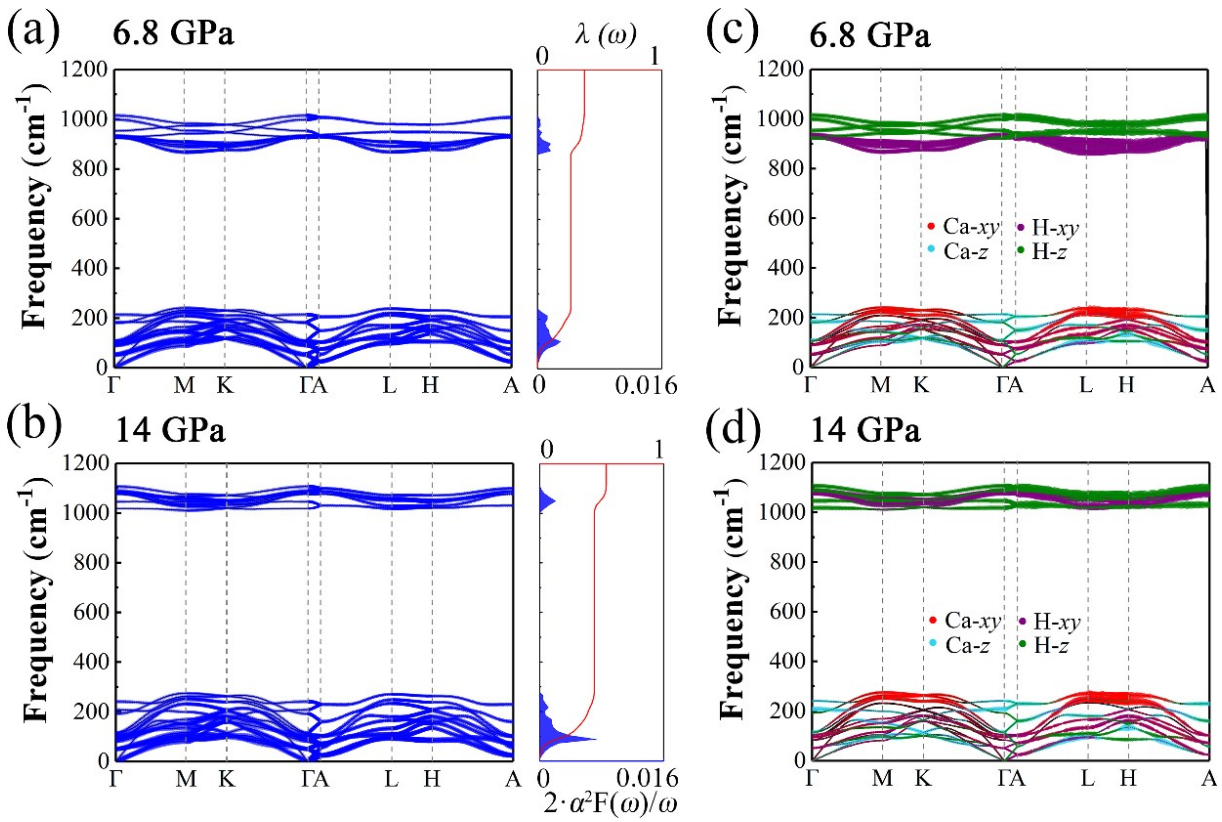

Fig. S9. Phonon dispersions weighted by the magnitude of the EPC, the mode-resolved Eliashberg spectral function $2 \cdot \alpha^2 F(\omega)/\omega$, and the frequency-dependent electron-phonon coupling parameters $\lambda(\omega)$ for Ca_3H_2 at (a) 6.8 GPa, and (b) 14 GPa. The sizes of blue dots are proportional to the phonon linewidth γ_{qv}. Phonon dispersions weighted by the vibrational modes of different atoms for Ca_3H_2 at (c) 6.8 GPa and (d) 14 GPa.

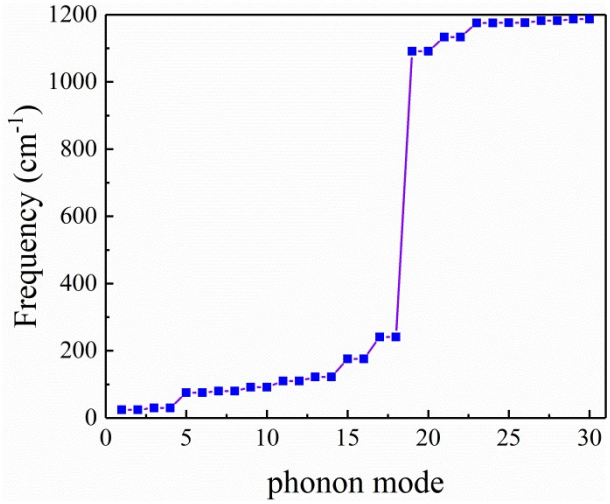

Fig. S10. The single *q*-point phonon test results.

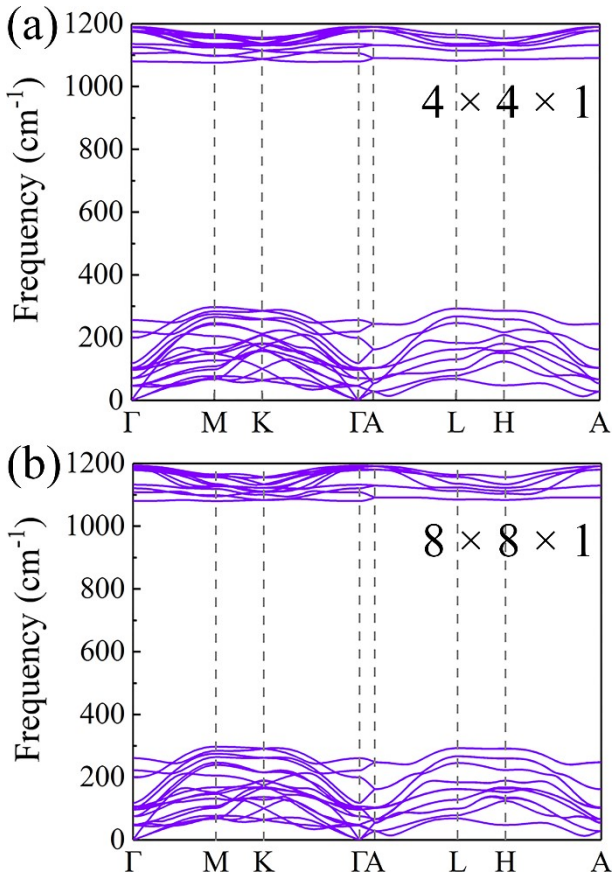

Fig. S11. Phonon dispersion comparison of Ca_3H_2 at different *q*-points of (a) 4 × 4 × 1, and (b) 8 × 8 × 1 under 19.5 GPa.

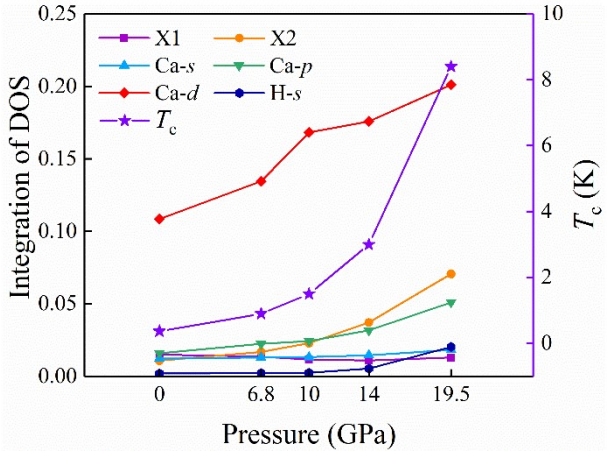

Fig. S12. Integration of density of states for interstitial anion electrons.

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