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

Supplementary information

Stable structures and superconductivity of At-H system at high pressure

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Table S1 Structure parameters of the stable phases for AtH_2 and AtH_4.

Structure Space Pressure	Parameters (Å, deg)	Atom	x	y	z
AtH_2	a=3.6443	H1	0.00000	-0.06722	-0.36522
Cmcm	b=9.4561	At1	0.00000	-0.64446	-0.75000
(50 GPa)	c=3.3341				
AtH_2	a=5.8264	H1	0.44361	0.25000	0.67874
Pnma	b=2.9241	H5	0.49799	0.75000	0.47529
(200 GPa)	c=4.5377	At1	0.17820	0.75000	0.64043
AtH_4	a=3.2725	H1	0.66667	0.33333	0.62953
*P*6/*mmm*	b=3.2725	At1	0.00000	0.00000	0.00000
(100 GPa)	c=3.0160				
	γ=120				
AtH_4	a= 4.9931	H1	-0.70156	0.00846	1.00000
Cmmm	b= 2.7459	At1	-0.50000	-0.50000	0.50000
(250 GPa)	c= 3.0599				

Table S2 The H-H distances of the H_2-units and the charge transferred from At to H in AtH_2 and AtH_4 which is represented by σ (*e*) based on the Bader charge analysis

	Atom	σ (*e*)	H-H distances (Å)
AtH_2 *Cmcm* (50 GPa)	At	-0.16	0.77
AtH_2 *Pnma* (200 GPa)	At	-0.25	0.78
AtH_4 *P6*/*mmm* (100 GPa)	At	-0.35	0.78
AtH_4 *Cmmm* (250 GPa)	At	-0.48	0.80

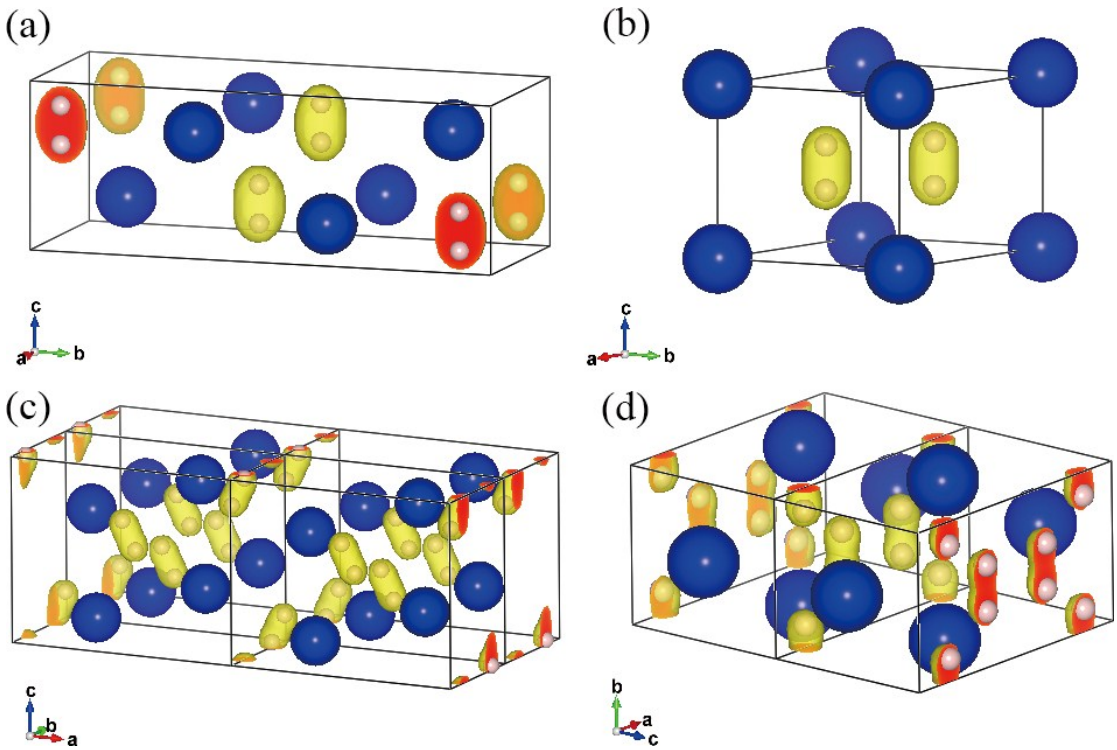

Fig. S1 The calculated electron localization function (ELF) for (a) *Cmcm*-AtH_2, (b) *Pnma*-AtH_2, (c) *P*6/*mmm*-AtH_4, (d) *Cmmm*-AtH_4. The isosurfaces are 0.9.

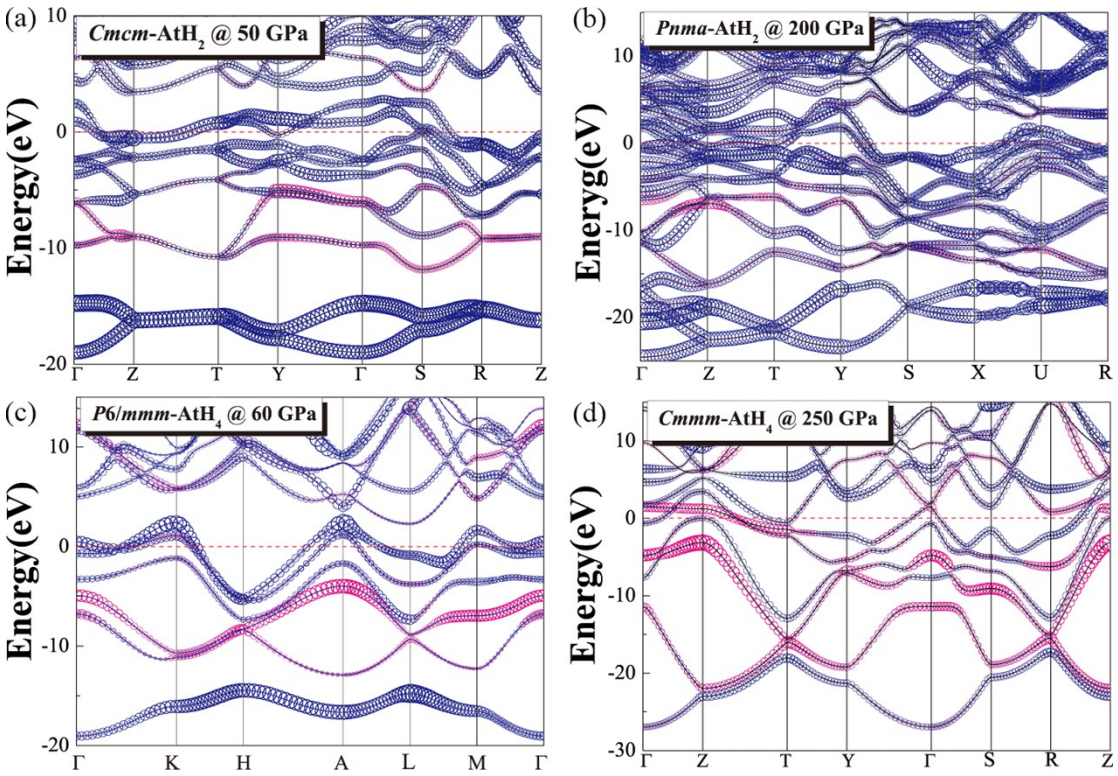

Fig.S2 Electronic band structure with the projection onto H atoms (magenta circles) and At atoms (blue circles) for (a) *Cmcm*-AtH_2 at 50 GPa. (b) *Pnma*-AtH_2 at 200 GPa, (c) *P*6/*mmm*-AtH_4 at 60 GPa, (d) *Cmmm*-AtH_4 at 250 GPa.

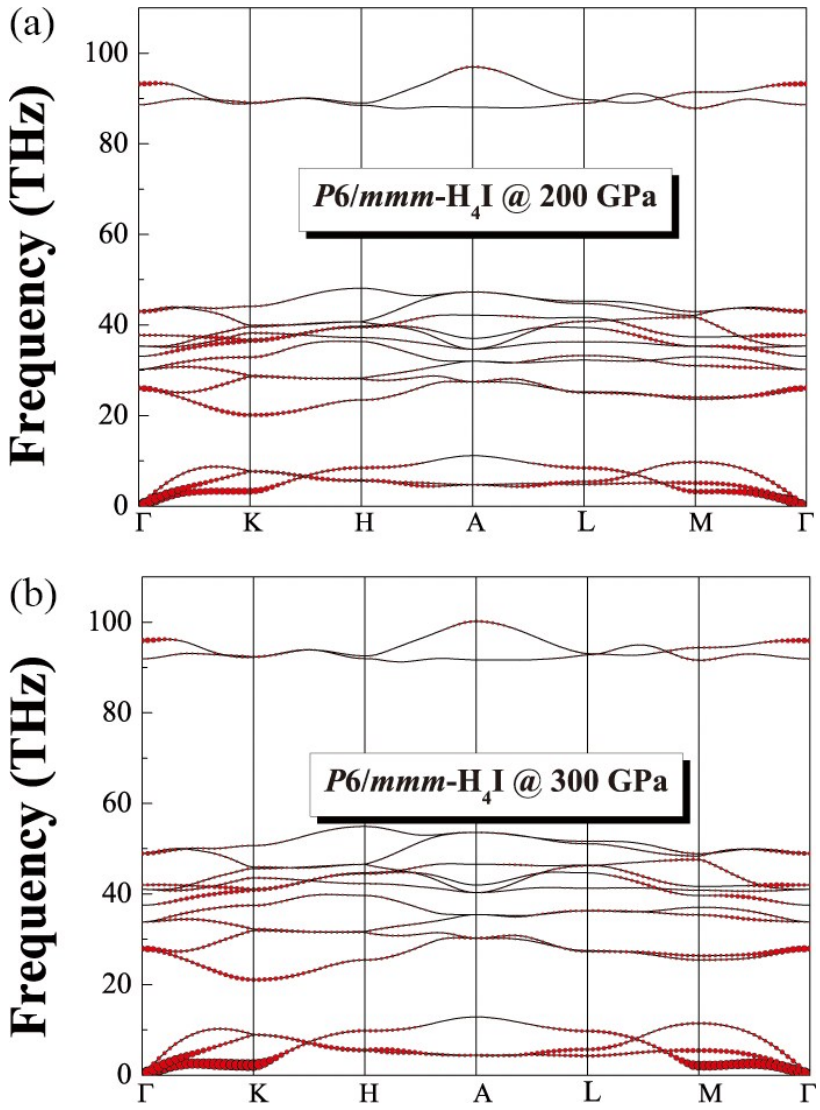

Fig.S3 (Color online) Phonon dispersion curves for *P*6/*mmm*-IH_4 at 200 GPa and 300 GPa with electron–phonon parameter $\lambda_{q,j}(\omega)$ of each mode (q, j). The red solid circles shown in the band structures indicate EPC with a radius proportional to their respective strength. A larger radius represents greater $\lambda_{q,j}(\omega)$.

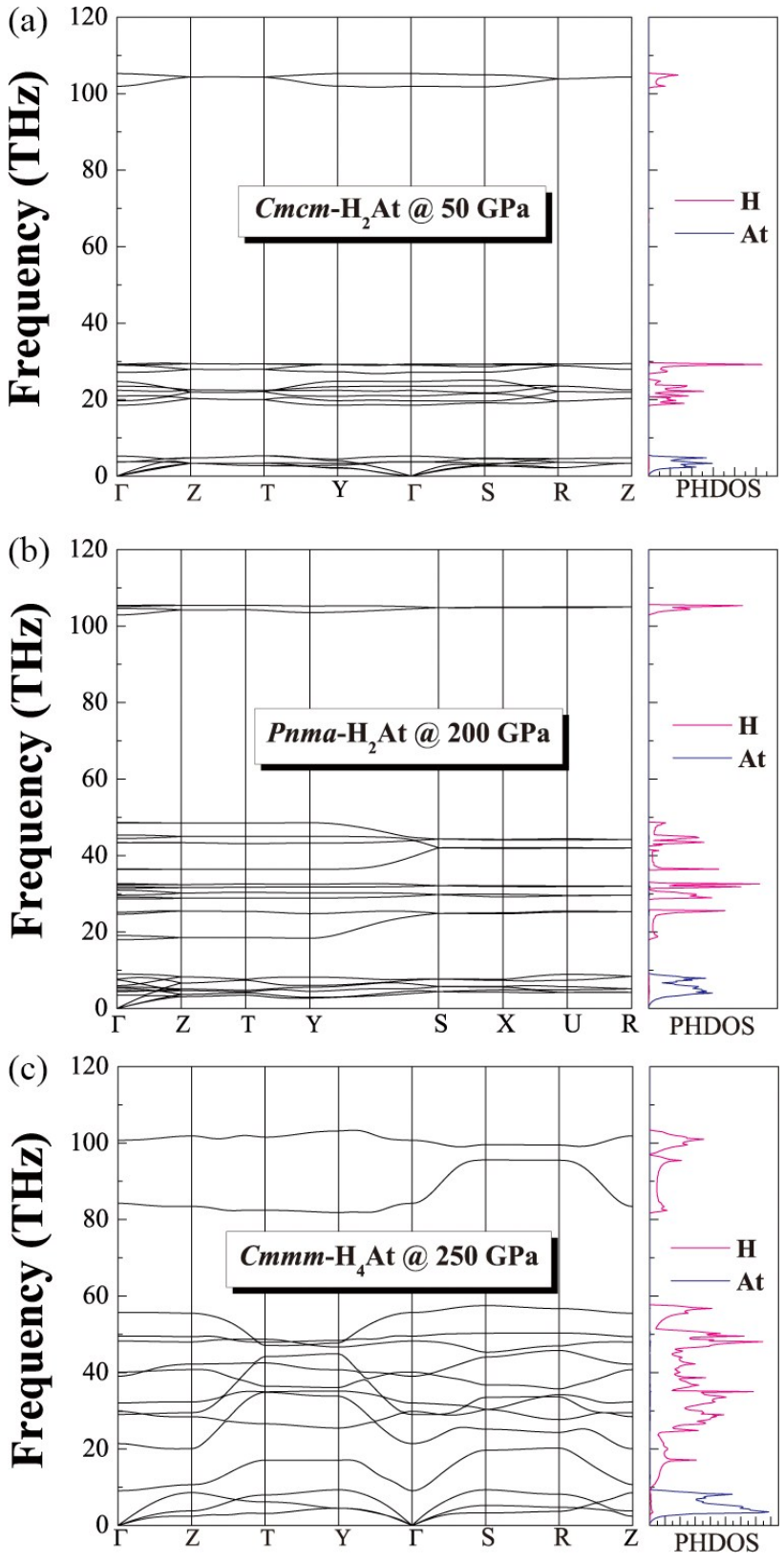

Fig. S4 Phonon dispersion curves, phonon density of states (PHDOS) projected on At and H atoms for (a) *Cmcm*-AtH_2 at 50 GPa. (b) *Pnma*-AtH_2 at 200 GPa, (c) *Cmmm*-AtH_4 at 250 GPa.