Supporting Information

First-principles study on the structures and superconductivity of H-S-La system under high pressure

*Yin L. Xu,[a] Yang M. Chen,[*a] Xiao Z. Yan,[*a] Yi B. Huang[a], Xing Z. Zhou[a], Quan X. Wu[a], Xiao W. Sheng [b, c] and Fang G. Kuang [d]*

a. School of Science, Jiangxi University of Science and Technology, Ganzhou 341000, Jiangxi, China.

b. Address here Department of Physics, Anhui Normal University, Anhui, Wuhu 241000, China

c. Anhui Province Key Laboratory of Optoelectric Materials Science and Technology, Wuhu 241000, China.

d. School of Physics and Electronic Information, Gannan Normal University, Ganzhou 341000, China

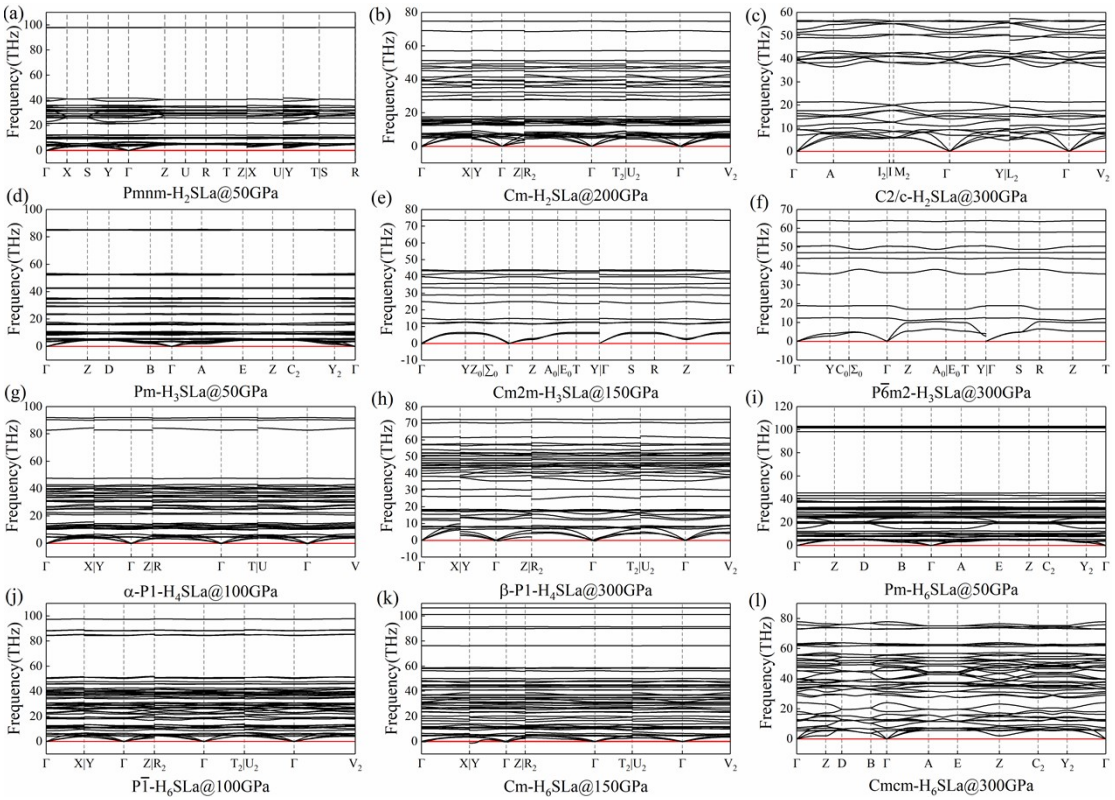

Fig. S1 Phonon dispersion curves (a) *Pmnm*-H_2SLa at 50 GPa (b) *Cm*-H_2SLa at 200 GPa (c) *C2/c*-H_2SLa at 300 GPa (d) *Pm*-H_3SLa at 50 GPa (e) *Cm2m*-H_3SLa at 150 GPa (f) $P\bar{6}m2$-H_3SLa at 300 GPa (g) α-*P1*-H_4SLa at 100 GPa (h) β-*P1*-H_4SLa at 300 GPa (i) *Pm*-H_6SLa at 50 GPa (j) $P\bar{1}$-H_6SLa at 100 GPa (k) *Cm*-H_6SLa at 150 GPa and (l) *Cmcm*-H_6SLa at 300 GPa

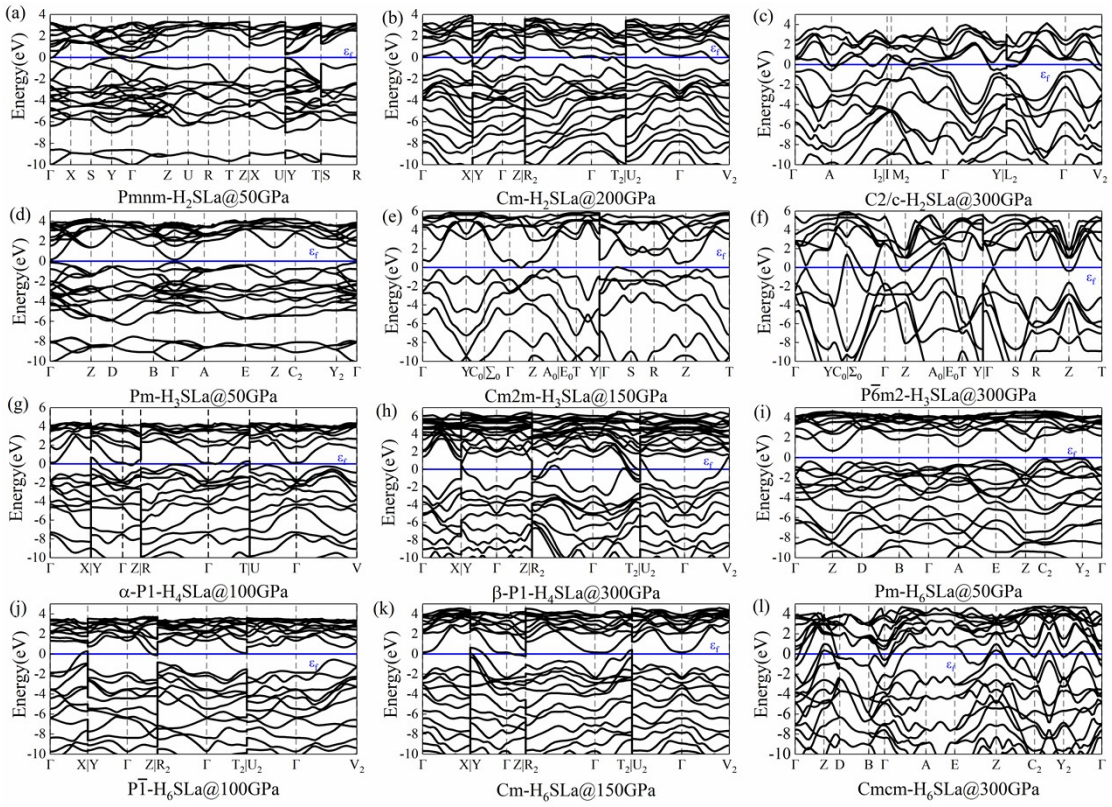

Fig. S2 Electronic band structures (a) *Pmnm*-H_2SLa at 50 GPa (b) *Cm*-H_2SLa at 200 GPa (c) *C2/c*-H_2SLa at 300 GPa (d) *Pm*-H_3SLa at 50 GPa (e) *Cm2m*-H_3SLa at 150 GPa (f) $P\bar{6}m2$-H_3SLa at 300 GPa (g) α-*P1*-H_4SLa at 100 GPa (h) β-*P1*-H_4SLa at 300 GPa (i) *Pm*-H_6SLa at 50 GPa (j) $P\bar{1}$-H_6SLa at 100 GPa (k) *Cm*-H_6SLa at 150 GPa and (l) *Cmcm*-H_6SLa at 300 GPa

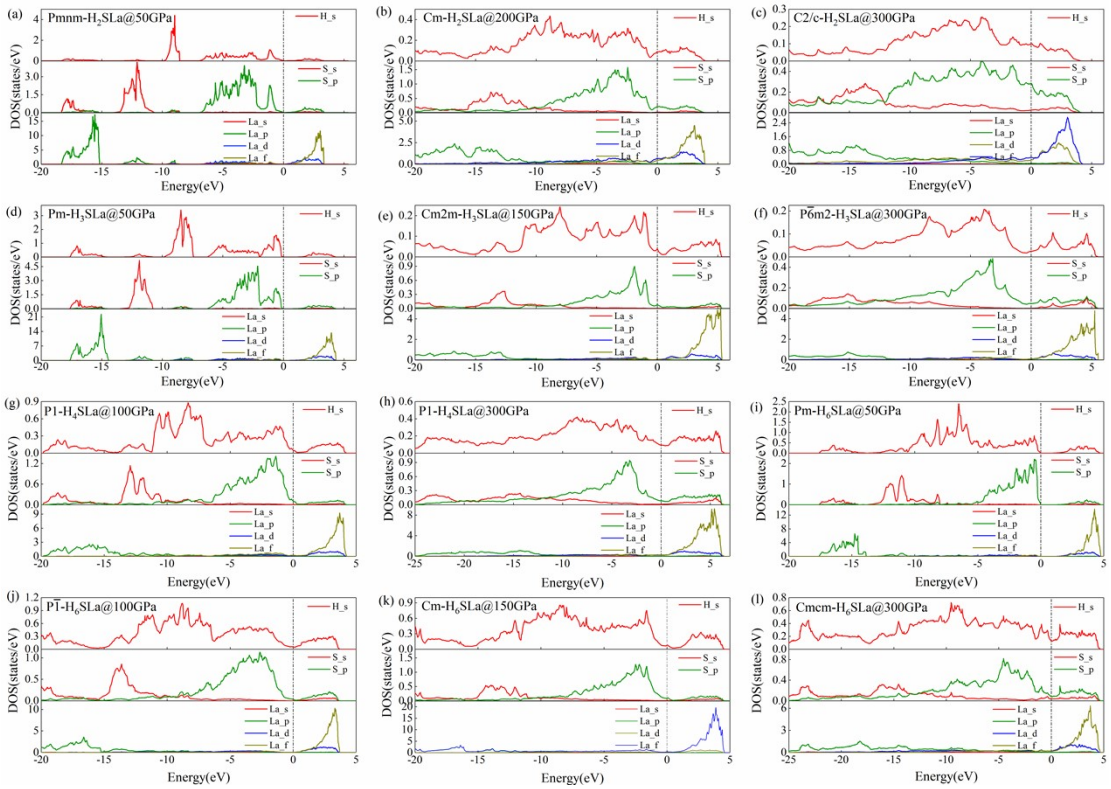

Fig. S3 Partial density of states (a) *Pmnm*-H_2SLa at 50 GPa (b) *Cm*-H_2SLa at 200 GPa (c) *C2/c*-H_2SLa at 300 GPa (d) *Pm*-H_3SLa at 50 GPa (e) *Cm2m*-H_3SLa at 150 GPa (f) $P\bar{6}m2$-H_3SLa at 300 GPa (g) α-*P1*-H_4SLa at 100 GPa (h) β-*P1*-H_4SLa at 300 GPa (i) *Pm*-H_6SLa at 50 GPa (j) $P\bar{1}$-H_6SLa at 100 GPa (k) *Cm*-H_6SLa at 150 GPa and (l) *Cmcm*-H_6SLa at 300 GPa

Table S1 Bader charge analysis of *Cm*-H_2SLa at 200 GPa.

Atom	Charge value/e	Charge transfer $\sigma(e)$
H1	1.005702	-0.005702
H2	1.279160	-0.279160
H3	1.232920	-0.232920
H4	1.074050	-0.074050
H5	1.121001	-0.121001
H6	0.966219	0.033781
S1	6.764084	-0.764084
S2	6.857769	-0.857769
S3	6.739494	-0.739494
La1	9.919119	1.080881
La2	10.051050	0.94895
La3	9.989432	1.010568

Table S2 Bader charge analysis of *C2/c*-H_2SLa at 300 GPa·

Atom	Charge value/e	Charge transfer $\sigma(e)$
H1	1.159932	-0.159932
H2	1.159932	-0.159932
H3	1.159815	-0.159815
H4	1.159815	-0.159815
S1	6.525008	-0.525008
S2	6.525008	-0.525008
La1	10.155245	0.844755
La2	10.155245	0.844755

Table S3 Bader charge analysis of *Cmcm*-H_6SLa at 300 GPa.

Atom	Charge value/e	Charge transfer $\sigma(e)$
H1	1.097159	-0.097159
H2	1.097159	-0.097159
H3	0.920404	0.079596
H4	0.920404	0.079596
H5	1.189627	-0.189627
H6	1.189388	-0.189388
H7	1.224568	-0.224568
H8	1.189388	-0.189388
H9	0.920404	0.079596
H10	1.224568	-0.224568
H11	0.920404	0.079596
H12	1.189627	-0.189627
S1	6.493544	-0.493544
S2	6.493544	-0.493544
La1	9.964905	1.035095
La2	9.964905	1.035095

Table S4 Lattice parameters and atomic positions for predicted H-S-La systems

Compound	Pressure GPa	Space group	Lattice parameters Å, degree	Atomic positions
H_2SLa	50	*Pmnm*	a=6.454	H 0.562 0.425 0.500
			b=6.593	H 0.937 0.574 0.000
			c=3.718	H 0.156 0.066 0.500
			α=β=γ=90	H 0.343 0.933 0.000
				H 0.656 0.933 0.000
				H 0.843 0.066 0.500
				H 0.062 0.574 0.000
				H 0.437 0.425 0.500
				S 0.774 0.713 0.500
				S 0.725 0.286 0.000
				S 0.225 0.713 0.500
				S 0.274 0.286 0.000
				La 0.500 0.626 0.000
				La 0.000 0.373 0.500
				La 0.000 0.936 0.000
				La 0.500 0.063 0.500
	200	*Cm*	a=2.851	H 0.575 0.150 0.649
			b=4.816	H 0.718 0.436 0.643
			c=6.125	H 0.206 0.412 0.215
			α=99.00	H 0.527 0.055 0.766
			β=89.99	H 0.728 0.456 0.343
			γ=107.22	H 0.675 0.351 0.452
				S 0.066 0.133 0.472
				S 0.918 0.836 0.833
				S 0.835 0.670 0.162
				La 0.349 0.699 0.505
				La 0.548 0.096 0.137
				La 0.195 0.391 0.864

	300	*C2/c*	a=3.687 b=c=3.703 α=102.95 β=γ=104.28	H 0.851 0.346 0.043 H 0.351 0.043 0.346 H 0.148 0.653 0.956 H 0.648 0.956 0.653 S 0.250 0.569 0.430 S 0.750 0.430 0.569 La 0.250 0.153 0.846 La 0.750 0.846 0.153
H_3SLa	50	*Pm*	a=7.053 b=3.53 c=6.809 α=β=γ=90	H 0.995 1.000 0.939 H 0.495 0.500 0.583 H 0.051 0.500 0.083 H 0.643 0.000 0.281 H 0.903 1.000 0.781 H 0.143 0.500 0.362 H 0.403 0.500 0.741 H 0.551 0.000 0.439 H 0.403 0.500 0.862 H 0.643 0.000 0.160 H 0.903 1.000 0.660 H 0.143 0.500 0.241 S 0.238 1.000 0.530 S 0.808 0.500 0.491 S 0.738 0.500 0.991 S 0.308 0.000 0.030 La 0.085 0.500 0.788 La 0.961 0.000 0.233 La 0.585 1.000 0.733 La 0.461 0.500 0.288
	150	*Cm2m*	a=2.853 b=2.881 c=3.961 α=68.67 β=γ=90	H 0.154 0.751 0.497 H 0.500 0.888 0.223 H 0.845 0.751 0.497 S 0.500 0.176 0.647 La -0.000 0.464 0.070
	300	$P\bar{6}m2$	a=b=2.718 c=3.756 α=β=90 γ=120	H 0.333 0.666 0.194 H 0.666 0.333 0.000 H 0.333 0.666 0.805 S 0.000 0.000 0.000 La 0.666 0.333 0.500
H_4SLa	100	*P1*	a=3.049 b=4.098 c=6.673 α=107.34 β=90.36 γ=111.47	H 0.867 0.608 0.271 H 0.819 0.520 0.626 H 0.554 0.578 0.536 H 0.961 0.795 0.107 H 0.308 0.585 0.482 H 0.787 0.443 0.944 H 0.743 0.360 0.814 H 0.931 0.694 0.401 S 0.118 0.108 0.651 S 0.243 0.356 0.102 La 0.462 0.801 0.860 La 0.597 0.065 0.336

	300	*P1*	a=3.692	H 0.592 0.344 0.527
			b=3.858	H 0.834 0.232 0.757
			c=3.894	H 0.854 0.738 0.257
			α=92.30	H 0.572 0.833 0.015
			β=γ=104.50	H 0.851 0.073 0.923
				H 0.015 0.944 0.631
				H 0.833 0.570 0.412
				H 0.077 0.466 0.646
				S 0.996 0.691 0.903
				S 0.001 0.194 0.350
				La 0.437 0.805 0.482
				La 0.432 0.298 0.987
H_6SLa	50	*Pm*	a=6.898	H 0.984 0.000 0.015
			b=3.410	H 0.319 -0.000 0.947
			c=4.560	H 0.028 0.500 0.221
			α=γ=90	H 0.599 0.000 0.384
			β=108.18	H 0.184 0.500 0.906
				H 0.106 -0.000 0.074
				H 0.771 0.000 0.142
				H 0.613 0.000 0.768
				H 0.906 0.500 0.183
				H 0.061 0.500 0.868
				H 0.491 0.000 0.705
				H 0.477 -0.000 0.320
				S 0.773 0.500 0.652
				S 0.317 0.500 0.437
				La 0.545 0.500 0.044
				La 0.045 0.000 0.544
	100	$P\bar{1}$	a=4.070	H 0.677 0.756 0.051
			b=4.154	H 0.564 0.061 0.535
			c=5.271	H 0.322 0.243 0.948
			α=111.15	H 0.782 0.872 0.896
			β=92.60	H 0.784 0.721 0.642
			γ=75.99	H 0.435 0.938 0.464
				H 0.507 0.813 0.154
				H 0.217 0.127 0.103
				H 0.875 0.755 0.516
				H 0.215 0.278 0.357
				H 0.124 0.244 0.483
				H 0.492 0.186 0.845
				S 0.890 0.274 0.753
				S 0.109 0.725 0.246
				La 0.713 0.311 0.238
				La 0.286 0.688 0.761

150	*Cm*	a=2.931	H 0.379 0.759 0.368
		b=3.918	H 0.363 0.727 0.476
		c=6.992	H 0.555 0.110 0.645
		α=102.18	H 0.962 0.924 0.188
		β=90	H 0.068 0.136 0.151
		γ=111.96	H 0.450 0.901 0.662
			H 0.960 0.921 0.360
			H 0.951 0.902 0.524
			H 0.866 0.732 0.584
			H 0.585 0.170 0.056
			H 0.680 0.360 0.831
			H 0.691 0.383 0.951
			S 0.208 0.417 0.654
			S 0.314 0.629 0.100
			La 0.970 0.941 0.872
			La 0.661 0.323 0.340
300	*Cmcm*	a=2.744	H 0.002 0.994 0.750
		b=3.641	H 0.997 0.005 0.250
		c=6.181	H 0.379 0.242 0.421
		α=β=90	H 0.620 0.757 0.921
		γ=67.88	H 0.252 0.495 0.454
			H 0.747 0.504 0.954
			H 0.580 0.838 0.750
			H 0.747 0.504 0.545
			H 0.620 0.757 0.578
			H 0.419 0.161 0.250
			H 0.379 0.242 0.078
			H 0.252 0.495 0.045
			S -0.000-0.000-0.000
			S -0.000-0.000 0.500
			La 0.295 0.408 0.750
			La 0.704 0.591 0.250