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

A unique metallic phase of the H_3S at high-pressure: Sulfur in three different local environments

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SUPLEMENTARY INFORMATION

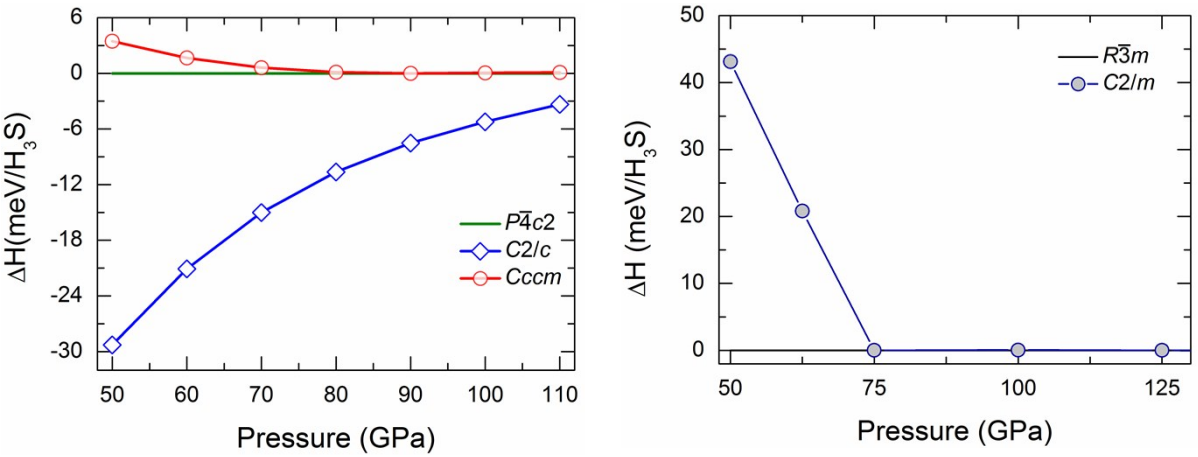


Figure 1S: Enthalpies of important structures below 100 GPa for H_3S.

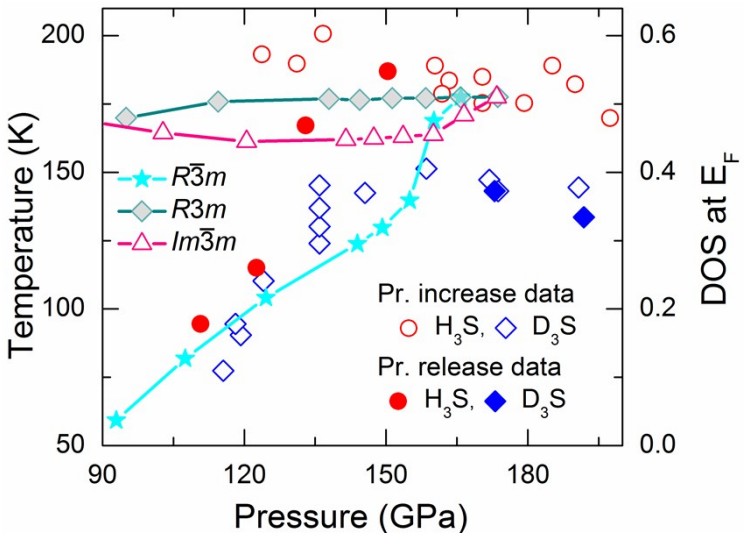


Figure 2S: Pressure variation of experimental superconducting temperature[1] and density of states at Fermi-level for $R3m$, $R\bar{3}m$ and $Im\bar{3}m$ phases (symbols with connecting lines). Open circles and diamonds show the experimental data taken during pressure increase. Filled circles and diamonds show the experimental data taken during pressure increase and decrease, respectively. Here, DOS is given in units of states/eV/H_3S.

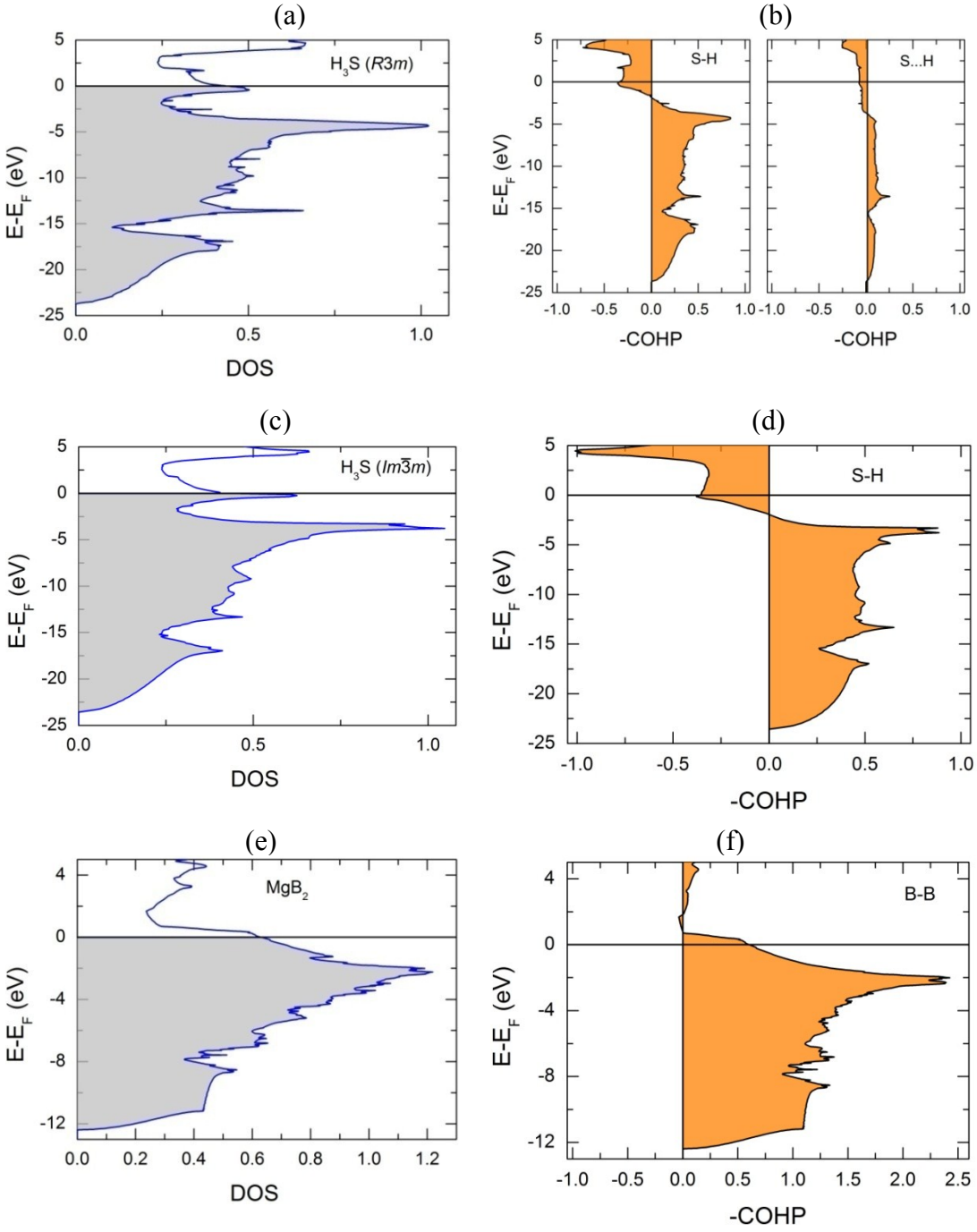


Figure 3S: (colour online) The COHP functions along with total DOS functions of H_3S and MgB_2. Here H_3S data is generated at 125 GPa and MgB_2 data is generated using ambient lattice parameters.

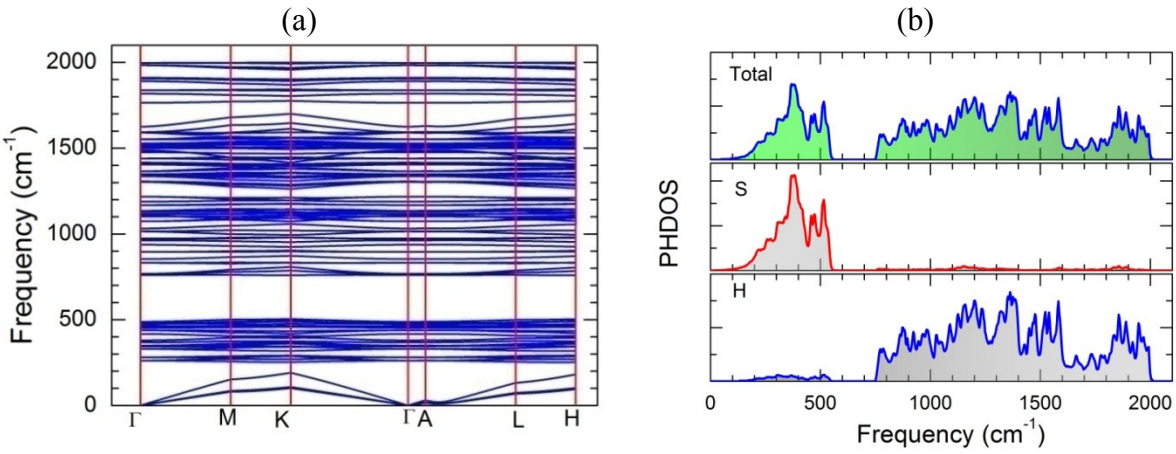
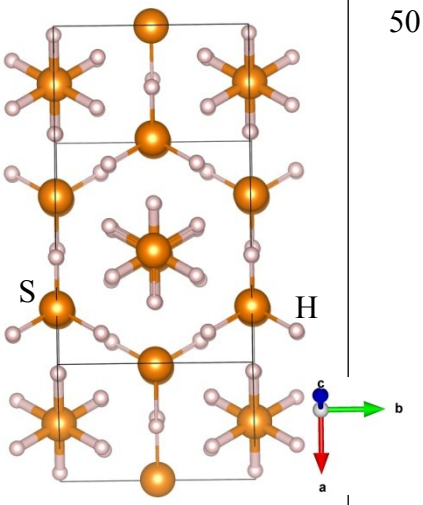
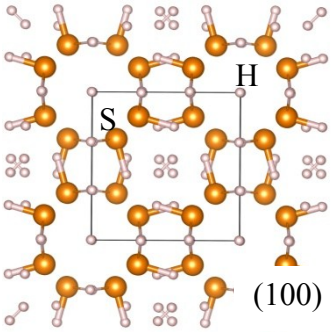


Figure 4S: Phonon properties of $R\bar{3}m$ phase of H_3S at 125 GPa. Here (a) shows the phonon dispersion curve and (b) shows projected phonon density of state functions.

Table IS: Crystallographic data of newly proposed H_3S structures as obtained in GGA calculations. Here pressure (P) is given in GPa unit and lattice parameters in angstrom unit.

	P	Lattice parameters	Atomic coordinates
$R\bar{3}m$	125	a = 4.3872 b = 4.3872 c = 22.1929	Hl (18*h*):0.48383 0.51617 0.06717 H2 (18*h*):0.84243 0.15757 0.22697 H3 (18*h*):0.17803 0.82197 0.01807 H4 (18*h*):0.48373 0.51627 0.19287 S1 (6*c*):0.00000 0.00000 0.06330 S2 (6*c*):0. 00000 0.00000 0.56250 S3 (6*c*):0. 00000 0.00000 0.68520 S4 (6*c*):0. 00000 0.00000 0.18960
*C*2/*m* 	50	a = 8.3767 b = 4.7401 c = 8.6491 β = 110.7890°	Hl (4*i*): -0.03653 0.00000 0.78249 H2 (4*i*): 0.45848 0.00000 0.28826 H3 (4*i*): 0.28088 0.00000 -0.03213 H4 (4*i*): 0.82559 0.00000 0.40894 H5 (8*j*): -0.06828 0.23621 0.06089 H6 (8*j*): 0.46424 0.29001 0.58749 H7 (8*j*): 0.32525 0.29089 0.20957 H8 (8*j*): 0.79343 0.20718 0.66287 S1 (4*i*): 0.44605 0.00000 0.81587 S2 (4*i*): -0.06970 0.00000 0.31279 S3 (4*i*): 0.83037 0.00000 -0.04902 S4 (4*i*): 0.31448 0.00000 0.42830
$P\bar{4}c2$ 	50	a = 5.8703 b = 5.8703 c = 4.9157	Hl (4*e*): 0.45517 0.45517 0.25000 H2 (8*j*): 0.01639 0.33494 0.26682 H3 (8*j*): 0.44999 0.77115 -0.00709 H4 (4*g*): 0.00000 0.00000 0.67283 S (8*j*): 0.68046 0.83552 -0.00751

References

1. M. Einaga, M. Sakata, T. Ishikawa, K. Shimizu, M. I. Eremets, A. P. Drozdov, I. A. Troyan, N. Hirao, and Y. Ohish, *Nat. Phys.*, 2016, **12 (9)**, 835.