Supplemental Material for

Predicted High-Temperature Superconductivity in Rare Earth Hydride ErH_2 at Moderate Pressure

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Table S1. The calculated elastic constants C_{ij} of ErH_2 under ambient pressures (in GPa) and the satisfaction with mechanical stability criteria (Y and N denote the satisfaction and the unsatisfaction, respectively).

P	C_{11}	C_{12}	C_{44}	Y/N
0	121.637	51.209	64.972	Y
6	158.495	59.177	54.465	Y
12	133.738	108.377	113.144	Y
14	145.060	101.757	253.158	Y
14.5	127.776	161.299	192.400	N
15	164.900	103.873	119.387	Y
16	148.068	126.347	76.245	N
18	176.988	105.421	-50.332	N
20	129.393	192.898	-24.491	N

The accompanying behaviors which could also to some extent support the affirmation of superconductivity at 15 GPa are presented in this Supplementary Materials. The calculated elastic constants C_{ij} under ambient pressures are presented in Table S1. Judged from the mechanical stability criterion,[1] this bulk became mechanical unstable at 14.5 GPa and up to 21.5 GPa except 15 GPa, as shown in Table S1. When the applied pressure was higher than 21.5 GPa, this bulk became lattice dynamical unstable, *i.e.*, imaginary frequency of phonon dispersions (not show) which is also the reason why the upper limit of the applied pressure in this work is 21.5 GPa. The mechanical stability criterion for cubic crystal could be expressed as:[1] $\tilde{C}_{44} > 0$, $\tilde{C}_{11} > |\tilde{C}_{12}|$, $\tilde{C}_{11} + 2\tilde{C}_{12} > 0$, where $\tilde{C}_{\alpha\alpha} = C_{\alpha\alpha} - P$ (α = 1, 4) and $\tilde{C}_{12} = C_{12} + P$, where P was the applied pressure. Meanwhile, superconductivity could also be reflected by an anomalous elastic softening over a temperature range for $PuCoGa_5$ which was a heavy fermion superconductor with T_c = 18.5 K.[2] Then, the analogous hopping of mechanical stability between 14.5 and 15 GPa of ErH_2 (Table S1) could also support the deduction of superconductivity at 15 GPa.

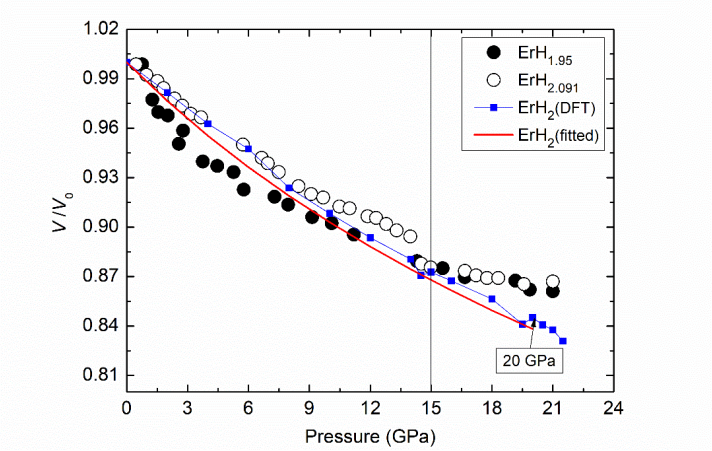

Fig. S1. The fitted normalized molar volumes (V/V_0) as a function of pressures for ErH_2 at 300 K (red solid line) using GIBBS thermodynamics scheme [3] with E-V data of DFT in this work. The corresponding relation calculated directly with DFT of this work is also plotted (blue solid line with square). The DAC data from Ref. [4] measured at room temperature for $ErH_{1.95}$ (solid circle) and $ErH_{2.091}$ (hollow circle) are also shown for comparison.

By means of Birch–Murnaghan Equation of State (EOS) fitting, the normalized molar volume (V/V_0) of ErH_2 at 300 K as a function of pressures (Fig. S1) is obtained by GIBBS thermodynamics scheme [3] using single point energy of unit cell (E) versus its volume (V) within DFT, *i.e.*, E-V curve which could be produced in this work (Fig. S2). The corresponding V/V_0 versus pressures relation calculated directly with DFT of this work is also plotted in Fig. S1. There is a tiny and clear deviation at this pressure away from the monotonous trend of the fitted curve in this work. Both the E-V data and the V/V_0 versus pressures relation of DFT have the same parameter settings and precision with the geometry optimizations of its unit cell (see the main text). The comparison with available experimental data for $ErH_{2.091}$ and $ErH_{1.95}$ measured at room temperature using diamond anvil cell techniques (DAC) [4] is also shown (Fig. S1)

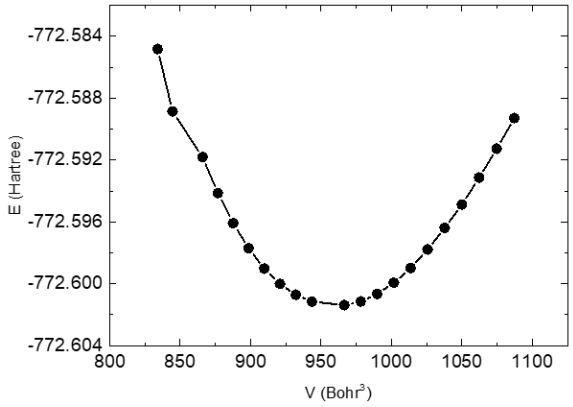

Fig. S2. The single point energy for unit cell (E) of ErH_2 versus its volume (V) within DFT.

The hypothesis of superconductivity at 20 GPa could also be supported by the tiny and clear deviation of the V/V_0 versus pressures relation calculated directly with DFT at this pressure away from the monotonous trend of the curve fitted with E-V data of this work (Fig. S2).

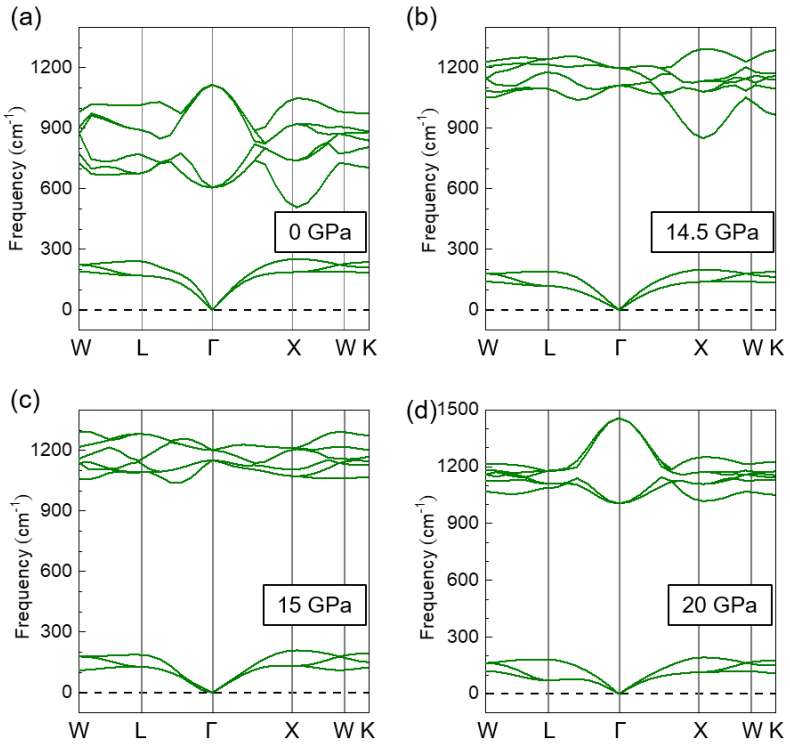

Fig. S3. The calculated phonon dispersions for ErH_2 at (a) 0, (b) 14.5, (c) 15, and (d) 20 GPa.

References

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