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

Supplementary Information for the paper entitled

"*Pressure-Induced Stability and Superconductivity in LuH_{12} polyhydrides*"

Junyi Du[†], Weiguo Sun[‡], Xiaofeng Li[‡], Feng Peng[‡,*]

[†] *School of Mathematical Sciences, Luoyang Normal University, Luoyang 471934, China*

[‡] *College of Physics and Electronic Information & Henan Key Laboratory of Electromagnetic Transformation and Detection, Luoyang Normal University, Luoyang 471934, China*

[*] fpeng@calypso.cn or fpeng@lynu.edu.cn

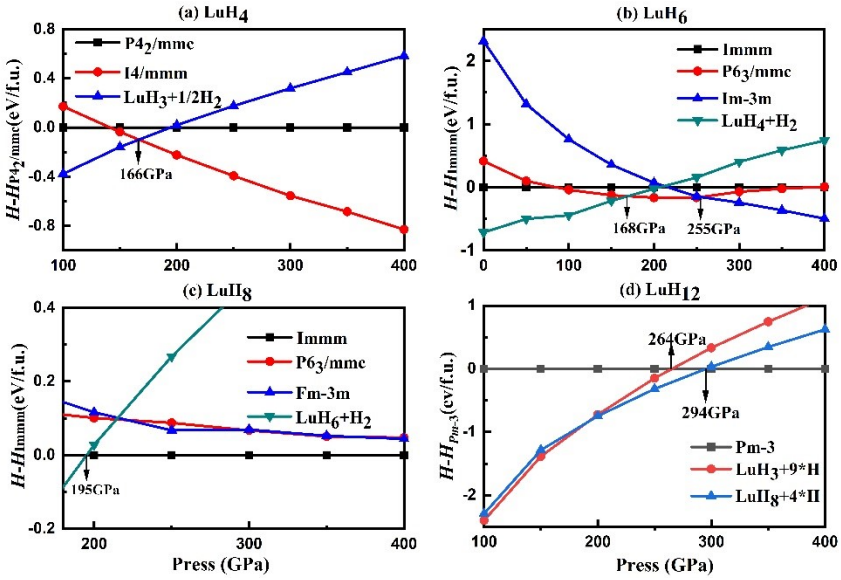

Fig.S1 The enthalpies difference of stable Lu-H compounds relative to other compounds and H_2 under pressure

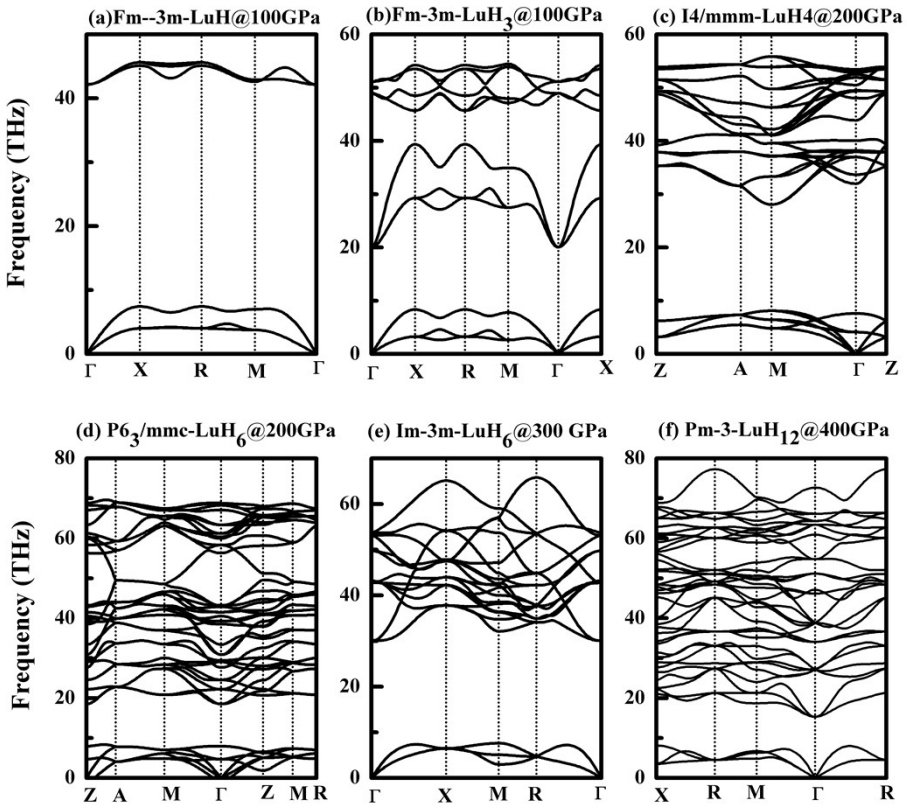

Fig.S2 The phonon dispersion curves of stable compounds.

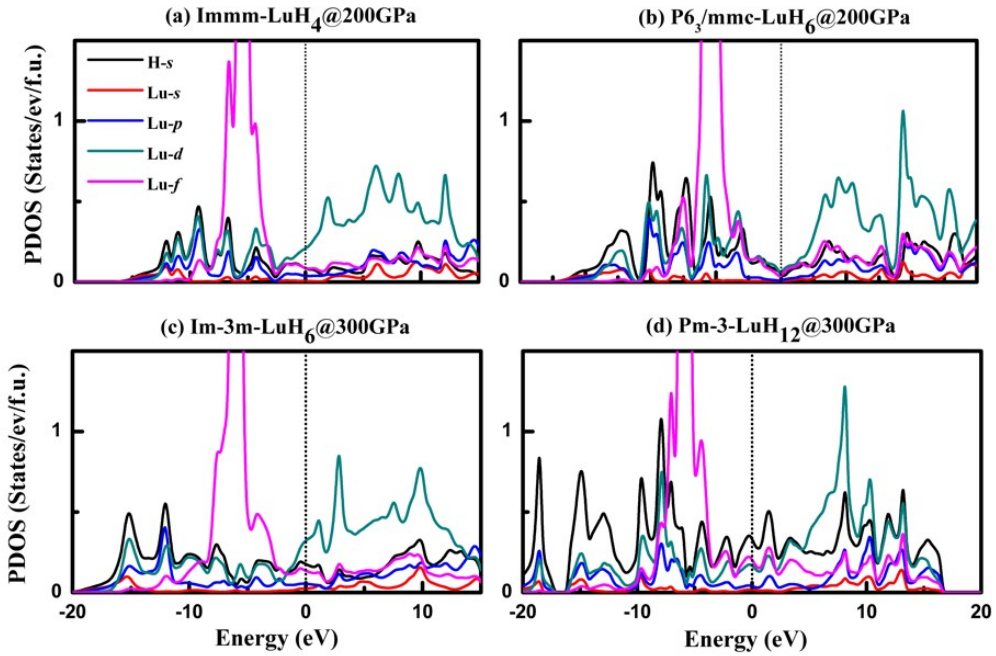

Fig.S3 The projected density of states of LuH_4, LuH_6 and LuH_{12}

Table S1 The crystal parameters of predicted stable lutetium polyhydrides

	Space group	Lattice parameters(Å)	Atoms	Atomic coordinates (fractional)		
				x	*y*	*z*
LuH (100GPa)	*Fm*-3*m*	*a*=*b*=*c*=4.033 *α*=*β*=*γ*=90º	Lu (4a) H (4a)	0.000 0.000	0.000 0.500	0.000 0.000
LuH_3 (100GPa)	*Fm*-3*m*	*a*=*b*=*c*=4.347 *α*=*β*=*γ*=90º	Lu (4a) H (4b) H (8c)	0.000 0.250 0.500	0.000 0.250 0.500	0.000 0.750 0.500
LuH_4 (200GPa)	*I*4/*mmm*	*a*=*b*=2.687 *c*=5.273 *α*=*β*=*γ*=90º	Lu (2a) H (4e) H (4d)	0.000 0.000 0.500	0.000 0.000 0.000	0.000 0.636 0.250
LuH_6 (200GPa)	$P6_3/mmc$	*a*=*b*=3.426 *c*=4.269 *α*=*β*=90º *γ*=120º	Lu (2d) H (12k)	0.333 0.839	0.667 0.161	0.750 0.875
LuH_6 (300GPa)	*Im*-3*m*	*a*=*b*=*c*=3.340 *α*=*β*=*γ*=90º	Lu (2a) H (12d)	0.000 0.000	0.000 0.750	0.000 0.500
LuH_8 (200GPa)	*Immm*	*a*=3.151 *b*=3.089 *c*=4.398 *α*=*β*=*γ*=90º	Lu (2a) H (8l) H (8m)	0.000 0.000 0.202	0.000 0.768 0.500	0.000 0.393 0.156
LuH_{12} (300GPa)	*Pm*-3	*a*=*b*=*c*=3.012 *α*=*β*=*γ*=90º	Lu (1b) H (12j)	0.500 0.668	0.500 0.788	0.500 0.000