Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information

Prediction of stoichiometric PoH_n compounds: crystal structures and properties

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Fig. S1: Fig. S1: the band structures of PoH-$P6_3/mmc$ and PoH_2-*Pnma* phases by GGA and hybrid functional HSE06 functions. (a) PoH-$P6_3/mmc$ at 300 GPa with GGA, (b) PoH-$P6_3/mmc$ at 300 GPa with HSE, (c) PoH_2-*Pnma* at 200 GPa with GGA, (d) PoH_2-*Pnma* at 200 GPa with HSE.

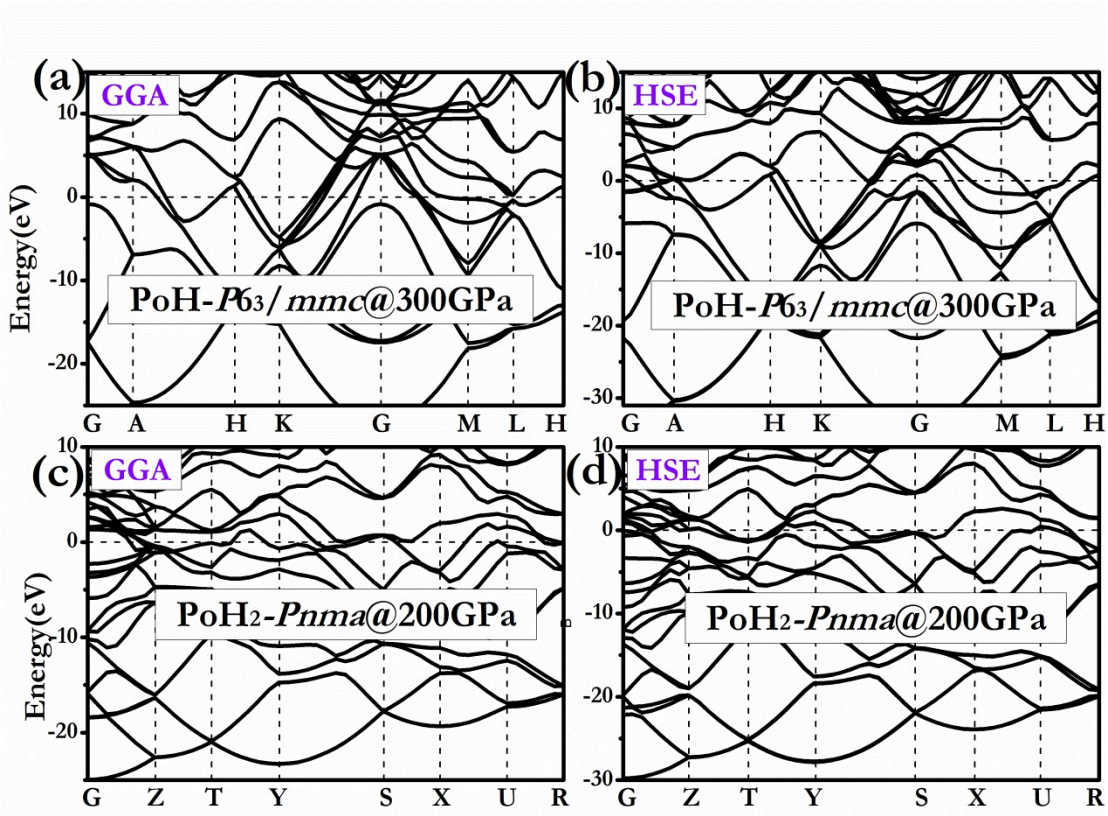

Table S1: Structural parameters of our predicted stable structures of Po-H system at selected pressure.

Space group Pressure	Lattice parameters (Å, °)	Atomic coordinates (fractional)	Sites
PoH-$P6_3/mmc$	a= b=2.8459	H1 0.0000 0.000 0.5000	2a
300 GPa	c=4.8312	Po1 0.3333 0.6667 0.2500	2c
	α=β= 90		
	γ=120		
PoH_2-*Cmcm*	a=3.2484	H1 0.1221 0.5485 0.7500	8g
50 GPa	b=9.8562	Po1 0.5000 0.6538 1.2500	4c
	c=3.3948		
	α=β=γ=90		
PoH_2-*Pnma*	a=5.2680	H1 0.5181 0.2500 0.0275	4c
300 GPa	b=2.8290	H5 0.4581 0.7500 0.7917	4c
	c=4.4494	Po1 0.1868 0.2500 0.8614	4c
	α=β=γ=90		
PoH_4-$C2/c$	a=4.0763	H1 -0.6353 -0.1896 -0.0539	8f
200 GPa	b=4.0845	H2 -0.1652 0.0541 -0.9026	8f
	c=7.8923	Po1 -0.5000 0.1046 -0.7500	4e
	α=γ=90		
	β=138.1964		
PoH_6-$C2/m$	a=12.1357	H1 -0.5308 0.3516 0.2507	8j
200 GPa	b=2.7962	H5 -0.7866 0.0000 0.8301	4i
	c=2.9633	H7 -0.7432 0.0000 0.1590	4i
	α=γ=90	H9 -0.1527 0.0000 0.2803	4i
	β=90.2911	H11 -0.2476 0.0000 0.5733	4i
		Po1 -0.6108 0.0000 0.7529	4i

Table S2 The calculated the logarithmic average phonon frequency ω_{log}, , electronic density of states at the Fermi level $N(E_f)$ (states/spin/Ry/Unit cell), electron-phonon coupling parameters (λ), and superconducting critical temperatures T_c of PoH_4-$C2/c$ at different pressures.

P(GPa)	ω_{log}(K)	N(ε_f)	λ	T_c(K)μ*=0.1	T_c(K)μ*=0.13
150	423.8	8.05	1.18	37.2	32.9
200	603	7.7	1.08	47.2	41.2
250	804.2	7.39	0.97	53.6	45.7