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

Supplementary Information for the paper entitled "*Crystal structures and superconductivity of Technetium Hydrides under Pressure*"

Xiaofeng Li[a], Hanyu Liu[b], Feng Peng[c,a]*

[a] *College of Physics and Electronic Information, Luoyang Normal College, Henan Luoyang, 471022, PR China*

[b] *Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, USA*

[c] *Beijing Computational Science Research Center, Beijing 100084, P. R. China.* *Email: fpeng@calypso.cn

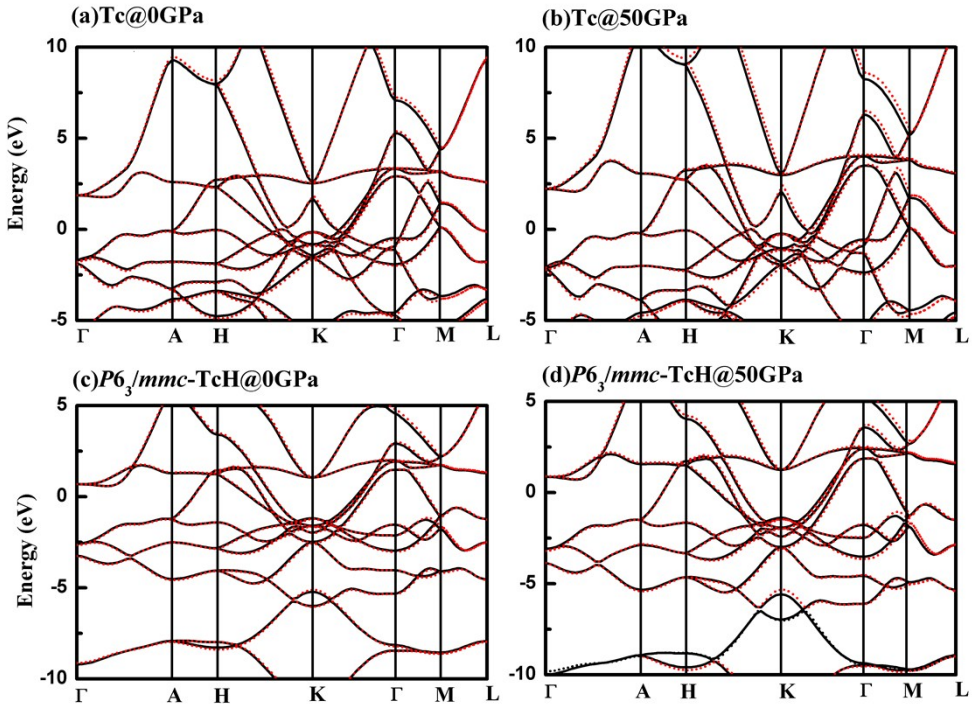

Fig. S1 The band structure of $P6_3/mmc$-Tc (a) 0GPa (b) 50GPa and $P6_3/mmc$-TcH (a) 0GPa (b) 50GPa. The black and red lines represented GGA and GGA+U, respectively.

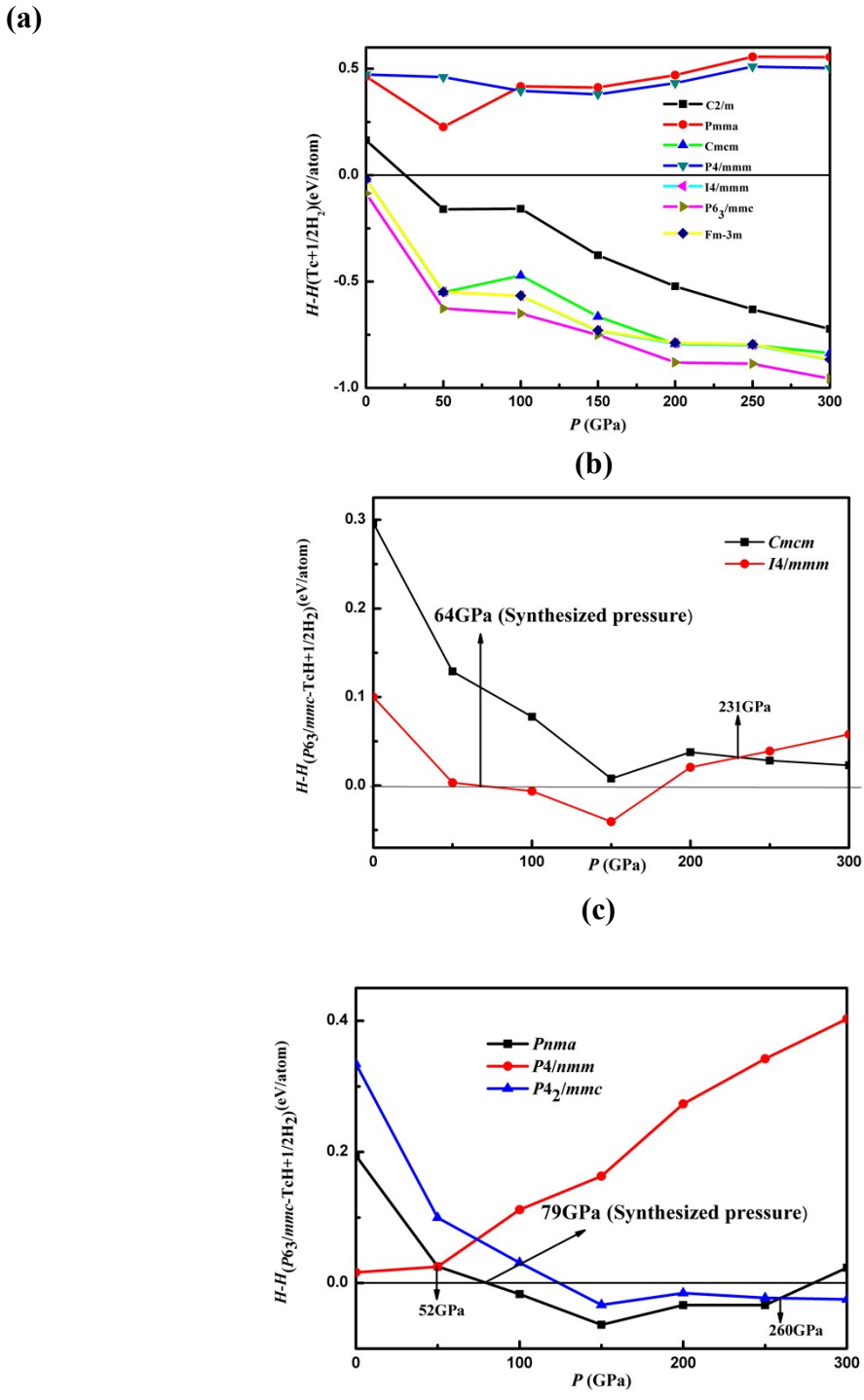

Fig.S2 Calculated enthalpies per atom of various structures in the pressure range of 0–300 GPa for (a) TcH with respect to 1/2H_2+Tc; (b) TcH_2 with respect to 1/2H_2+TcH; (c) TcH_3 with respect to 3/2H_2+TcH.

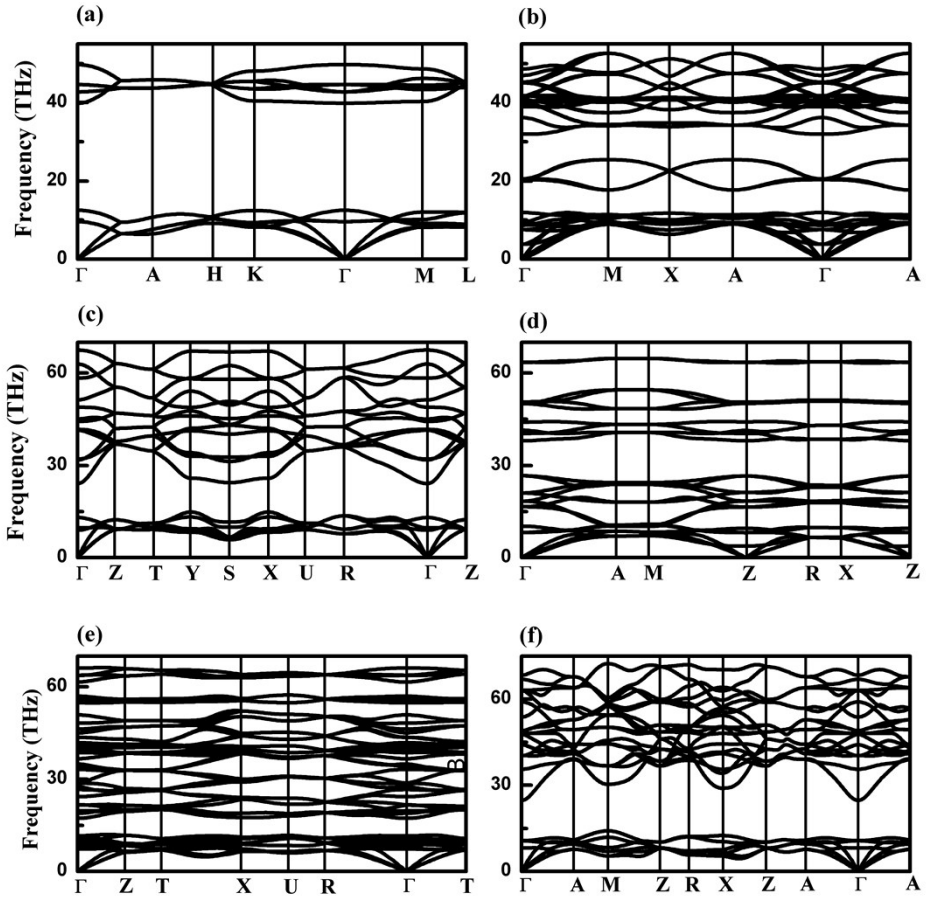

Fig S3 The phonon band structure (a) $P6_3/mmc$-TcH at 150GPa; (b) $I4/mmm$-TcH_2 at 200GPa; (c) $Cmcm$-TcH_2 at 300GPa; (d) $P4/nmm$-TcH_3 at 30GPa; (e) $Pnma$-TcH_3 at 150GPa; (f) $P4_2/mmc$-TcH_3 at 300GPa.

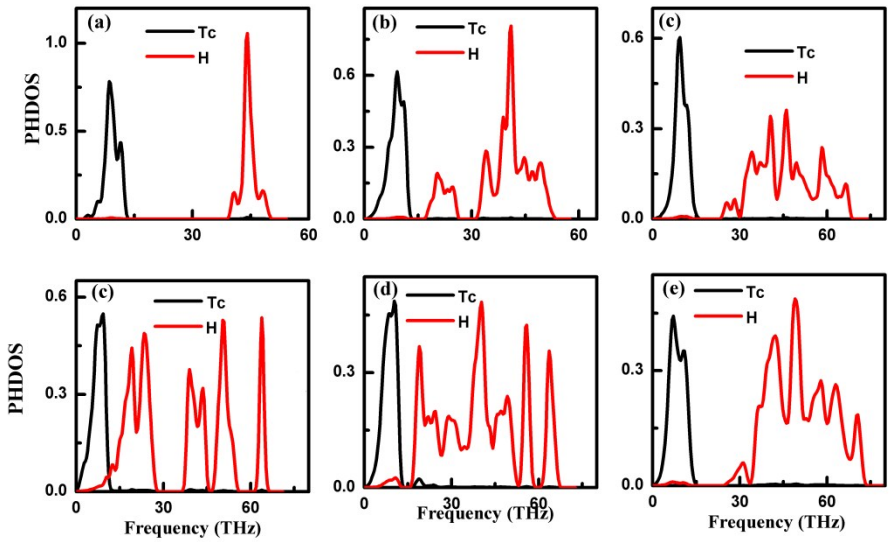

Fig S4 The projected phonon DOS (a) $P6_3/mmc$-TcH at 150GPa; (b) $I4/mmm$-TcH_2 at 200GPa; (c) $Cmcm$-TcH_2 at 300GPa; (d) $P4/nmm$-TcH_3 at 30GPa; (e) $Pnma$-TcH_3 at 150GPa; (f) $P4_2/mmc$-TcH_3 at 300GPa.

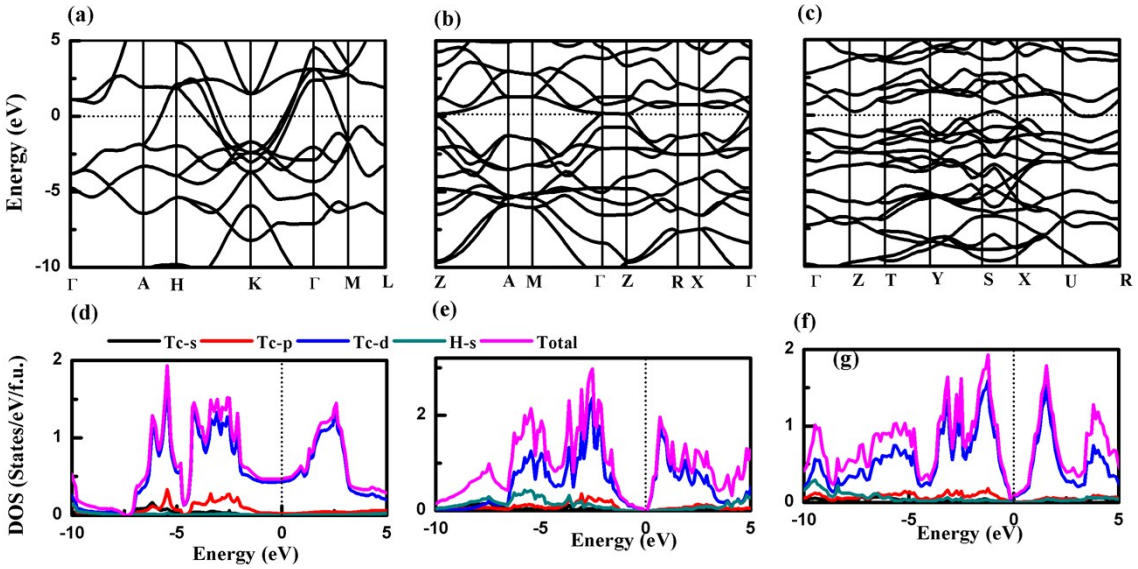

Fig.S5. Electronic band structure and density of states for (a, d) *P*6$_3$/*mmc*-TcH at 150GPa; (b, e) *P*4/*nmm*-TcH_3 at 30GPa; (c, f) *Pnma*-TcH_3 at 150GPa.

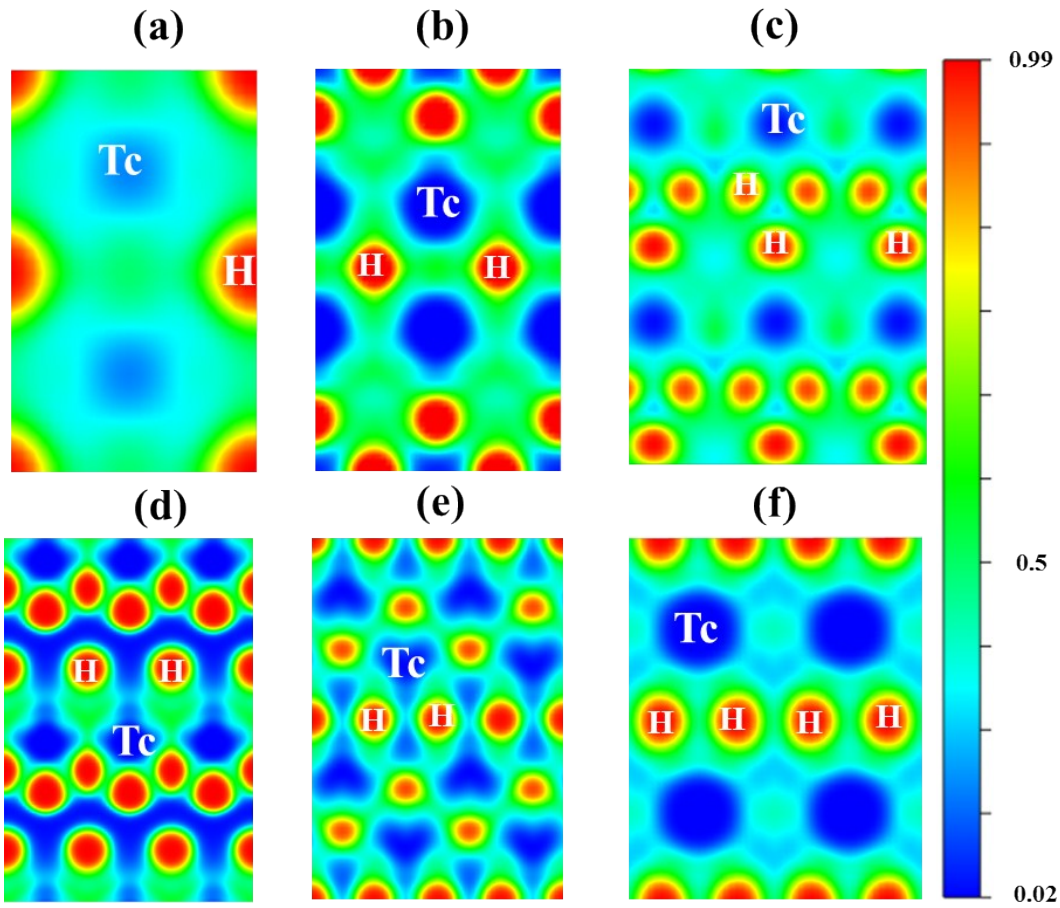

Fig.S6.Electron localization function (ELF) maps along (100) plane of (a) $P6_3/mmc$-TcH at 150GPa; (b) $I4/mmm$-TcH_2 at 200GPa; (c) $Cmcm$-TcH_2 at 300GPa; (d) $P4/nmm$-TcH_3 at 30GPa; (e) $Pnma$-TcH_3 at 150GPa; (f) $P4_2/mmc$-TcH_3 at 300GPa.

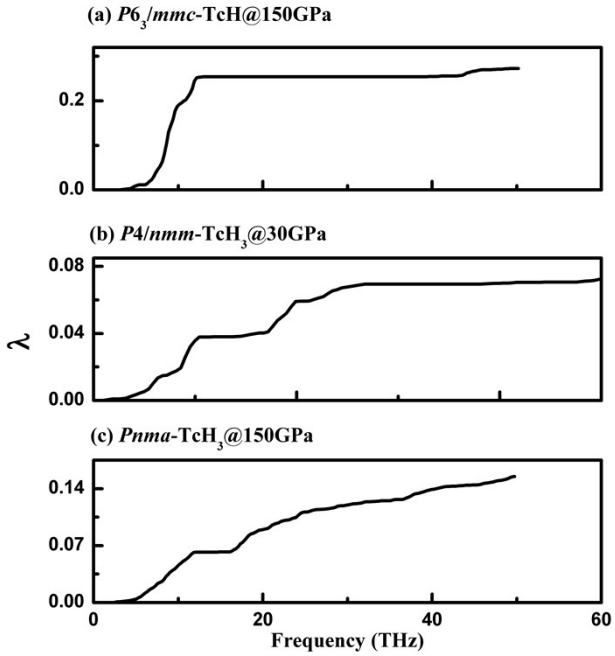

Fig.S7 EPC parameters of (a) $P6_3/mmc$-TcH at 150GPa; (b) $P4/nmm$-TcH_3 at 30GPa; (c) *Pnma*-TcH_3 at 150GPa.

Table S1 The calculated lattice constants of $P6_3/mmc$-Tc and $P6_3/mmc$-TcH with GGA and GGA+U

Phases		Pressure(GPa)	Lattice constants (Å)
Tc-$P6_3/mmc$	GGA	0	a=b=2.731; c=4.369
	GGA+U	0	a=b=2.744; c=4.376
Tc-$P6_3/mmc$	GGA	50	a=b=2.615; c=4.184
	GGA+U	50	a=b=2.630; c=4.210
TcH-$P6_3/mmc$	GGA	0	a=b=2.860; c=4.497
	GGA+U	0	a=b=2.872; c=4.512
TcH-$\boldsymbol{P6_3/mmc}$	GGA	50	a=b=2.736; c=4.300
	GGA+U	50	a=b=2.751; c=4.322

Table S2 Detailed structural information of the predicted stable Tc-H compounds at selected pressures.

Phases	Pressure (GPa)	Lattice constants (Å, º)	Atomic coordinates (fractional)			
TcH-$P6_3/mmc$	150	$a=b$=2.617	Tc(2c)	0.333	0.667	0.250
		c=4.133	H (2a)	0.000	0.000	0.000
		$\alpha=\beta$=90				
		γ=120				
TcH_2-I4/mmm	150	$a=b$=2.591	Tc(4e)	0.500	0.500	0.849
		c=8.540	H (4c)	0.500	0.000	0.000
		$\alpha=\beta=\gamma$=90	H (4e)	0.000	0.000	0.129
TcH_2-Cmcm	300	a= 2.504	Tc(4c)	0.500	0.863	0.750
		b= 7.780	H (4c)	0.500	0.648	0.750
		c= 2.483	H (4a)	0.500	0.500	0.000
		$\alpha=\beta=\gamma$=90				
TcH_3-P4/nmm	30	$a=b$=2.835	Tc(2c)	0.000	0.500	0.857
		c=8.540	H (2c)	0.000	0.500	0.571
		$\alpha=\beta=\gamma$=90	H (4f)	0.000	0.000	0.676
TcH_3-Pnma	150	a= 4.854	Tc(4c)	0.317	0.250	0.854
		b= 3.402	H (4c)	0.116	0.250	0.431
		c= 3.884	H (4c)	0.662	0.750	0.739
		$\alpha=\beta=\gamma$=90	H (4a)	0.000	0.500	0.000
TcH_3-$P4_2/mmc$	300	$a=b$=3.207	Tc(2c)	0.000	0.500	0.500
		c=2.643	H (4m)	0.500	0.702	0.500
		$\alpha=\beta=\gamma$=90	H (2e)	0.000	0.000	0.250