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

Supplementary Information for the paper entitled "Phase diagram and Superconductivity of Compressed Zirconium Hydrides"

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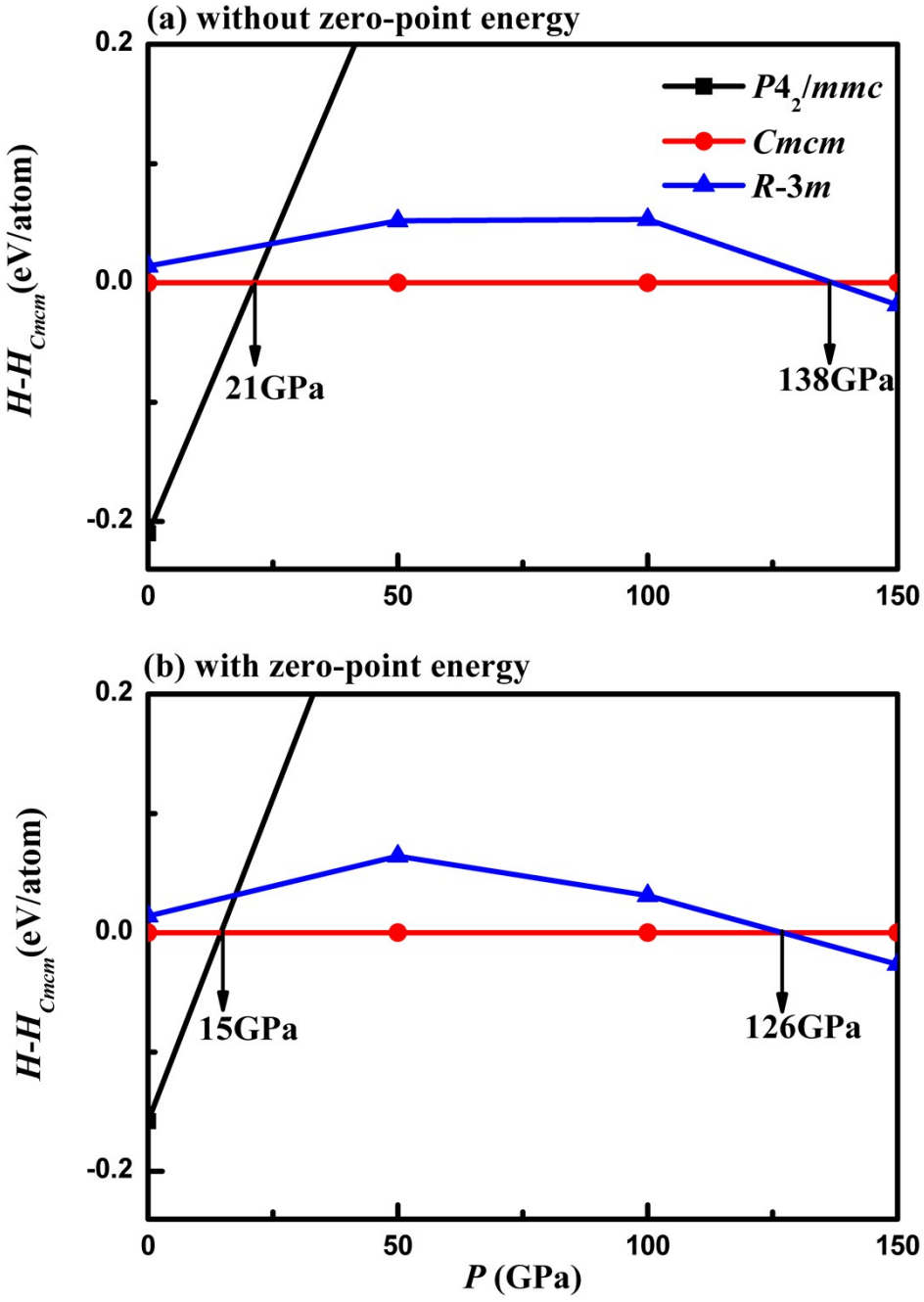

Figure S1 Calculated enthalpies per atom of various structures for ZrH in the pressure with respect to Cmcm phase without (a) and with (b) the inclusion of zero-point energy contribution.

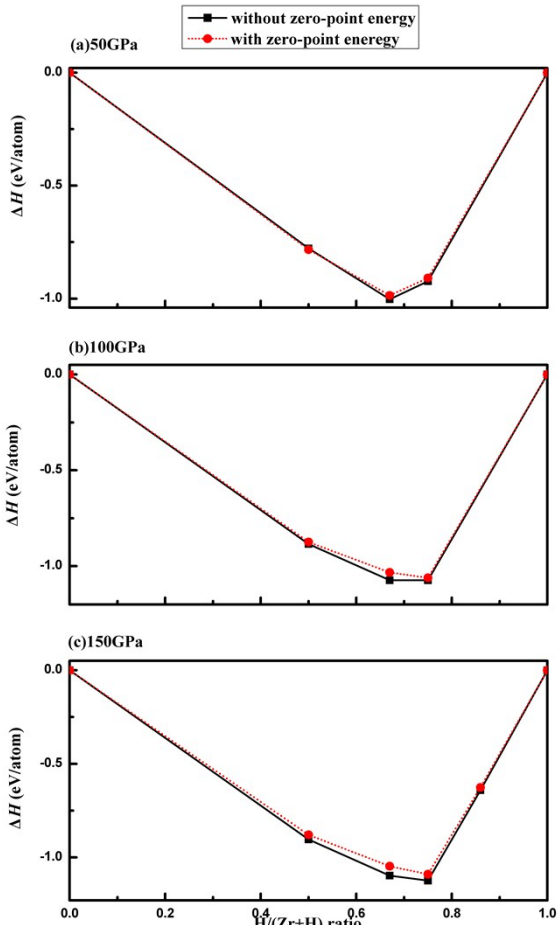

Figure S2. Relative formation enthalpies of the uncovered stable stoichiometries, e.g. ZrH, ZrH_2, ZrH_3 and ZrH_6 at 50,100 and 150 GPa with (short dot lines) and without (solid lines) the inclusion of zero-point energy contribution. One clearly sees that the introduction of zero-point energy does not change the essential energetic stabilities of these stable stoichiometries.

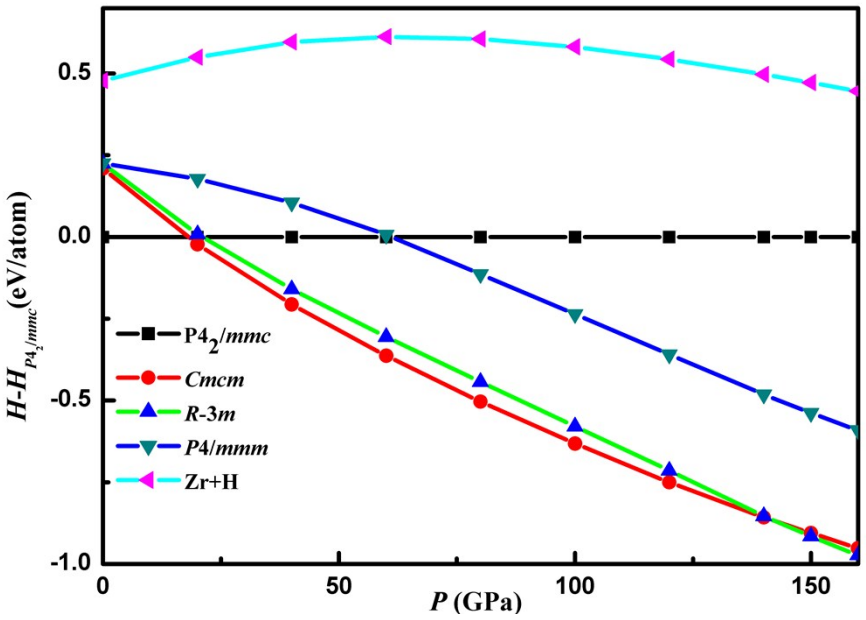

Figure S3 Calculated enthalpies per atom of various structures for ZrH in the pressure range of 0–160 GPa with respect to $P4_2$/mmc phase.

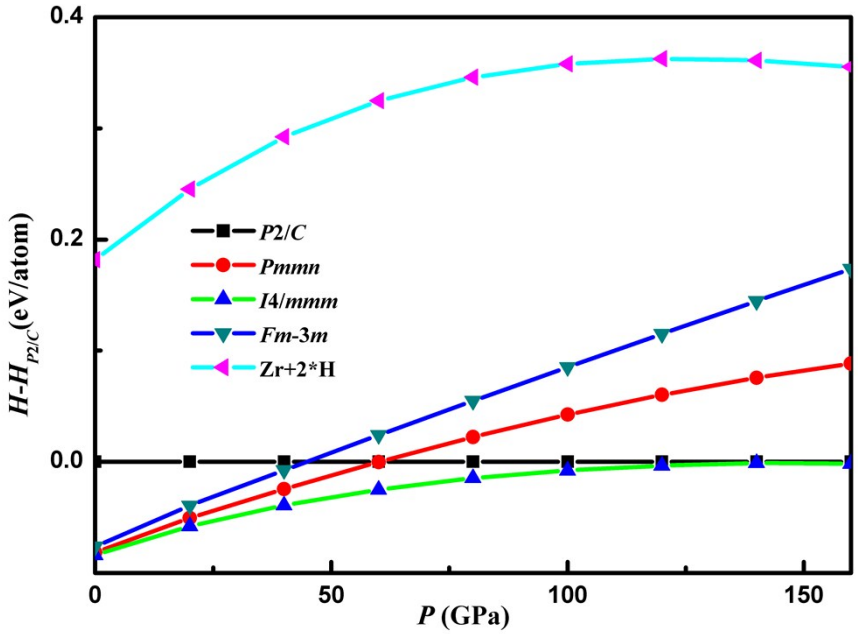

Figure S4 Calculated enthalpies per atom of various structures for ZrH_2 in the pressure range of 0–160 GPa with respect to P2/c phase.

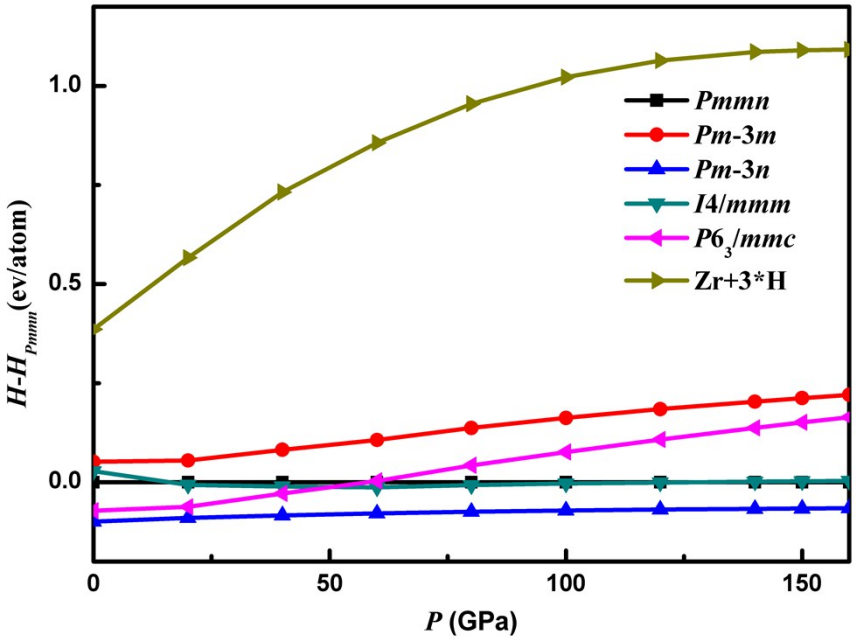

Figure S5 Calculated enthalpies per atom of various structures for ZrH_3 in the pressure range of 0–160 GPa with respect to Pmmn phase.

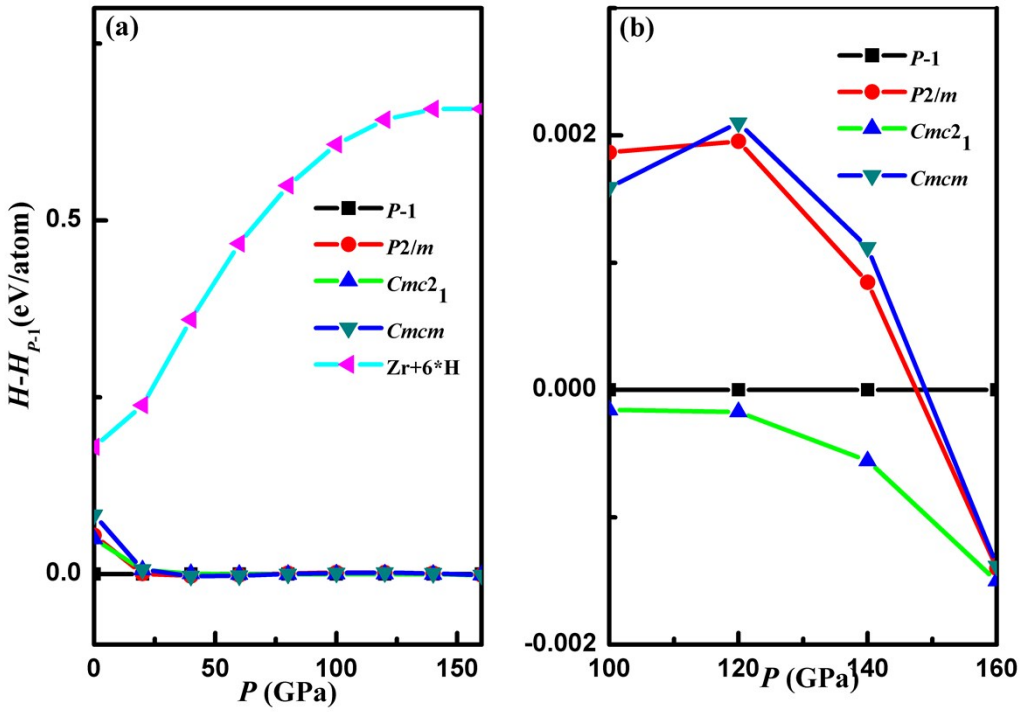

Figure S6 The left diagram is calculated enthalpies per atom of various structures for ZrH_6 in the pressure range of 0–160 GPa with respect to P-1 phase; The right diagram is the enthalpies differences compared to P-1 phase from 100GPa to 160GPa.

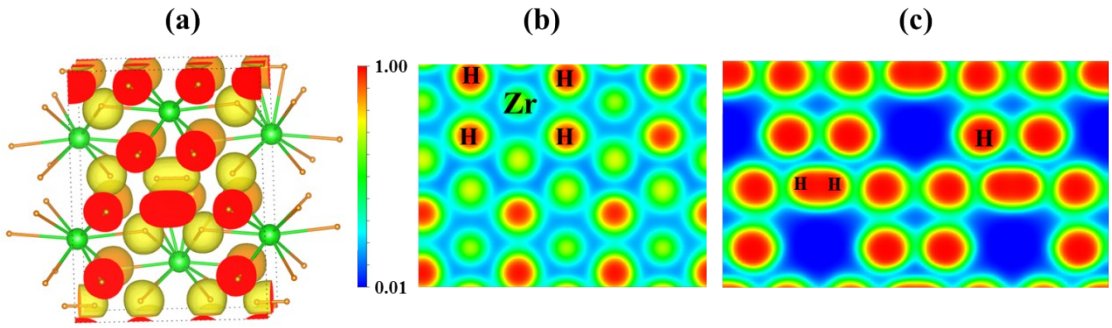

Figure S7 Calculated ELF of *Cmc*2_1-ZrH_6 with isosurface value of 0.8, (b) and (c) represented (100) and (001) planes, respectively.

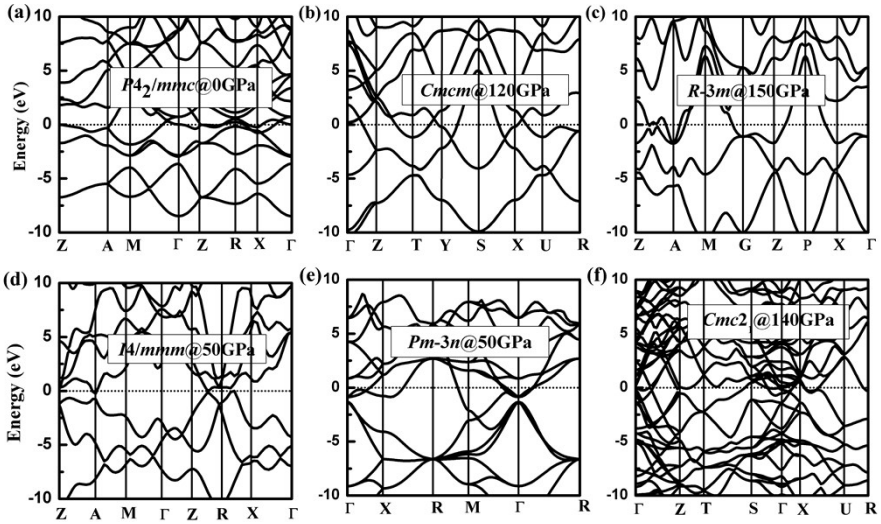

Figure S8 (a−f) Electronic band structures of the $P4_2/mmc$-ZrH, $Cmcm$-ZrH, R-3m-ZrH, $I4/mmm$-ZrH_2, Pm-3n-ZrH_3, and $Cmc2_1$-ZrH_6 at different pressures. The vertical dashed line at zero is the Fermi energy level.

Table S1 Detailed structural information of the predicted stable H-Se compounds at selected pressures.

Phases	Pressure (GPa)	Lattice constants (Å, º)	Atomic coordinates (fractional)			
ZrH-$P4_2/mmc$	0	$a=b$=3.241	Zr(2d)	0.500	0.000	0.000
		c=4.996	H (2e)	0.000	0.000	0.250
		$\alpha=\beta=\gamma$=90				
ZrH-$Cmcm$	120	a= 4.105	Zr(4c)	0.500	0.7502	0.750
		b=4.112	H (4c)	0.500	0.7488	0.250
		c=3.672				
		$\alpha=\beta=\gamma$=90				
ZrH-R-3m	150	$a=b$=2.893	Zr(3a)	0.000	0.000	0.000
		c=5.972	H (3b)	0.000	0.000	0.500
		$\alpha=\beta$=90				
		γ=120				
ZrH_2-$I4/mmm$	50	$a=b$=3.376	Zr(2b)	0.000	0.000	0.500
		c=3.784	H (4d)	0.000	0.500	0.250
		$\alpha=\beta=\gamma$=90				
ZrH_3-Pm-3n	50	$a=b=c$=3.572	Zr(2a)	0.000	0.000	0.000
		$\alpha=\beta=\gamma$=90	H (6c)	0.250	0.000	0.500
ZrH_6-$Cmc2_1$	140	a=5.119	Zr(4a)	0.000	0.788	0.039
		b=6.682	H (8b)	0.578	0.456	0.029
		c=2.791	H (8b)	0.853	0.838	0.538
		$\alpha=\beta=\gamma$=90	H (8b)	0.818	0.559	0.539