Supporting Information

Stability and Property of Ru-H System at High Pressure

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Table S1. Calculated structural parameters of our predicted stable structures for Ru-H system at their corresponding pressures.

Space group Pressure	Lattice parameters (Å, °)	Atomic coordinates (fractional)			Sites
$Fm\bar{3}m$-RuH	a=3.7267	H1 -0.50000	0.50000	0.50000	4b
100GPa	b=3.7267	Ru1 0.00000	0.00000	0.00000	4a
	c=3.7267				
	α=β=γ=90				
$Pm\bar{3}m$-RuH_3	a=2.598	H1 0.00000	0.00000	0.50000	3d
100 GPa	b=2.598	Ru1 0.50000	0.50000	0.50000	1b
	c=2.598				
	α=β=γ=90				
$Pm\bar{3}n$-RuH_3	a=3.1008	H1 0.00000	0.50000	0.25000	6c
200 GPa	b=3.1008	Ru1 0.00000	0.00000	0.00000	2a
	c=3.1008				
	α=β=γ=90				
*P*m-OsH_6	a=4.87	H1 0.29423	0.79604	0.27701	2c
50 GPa	b=5.6495	H2 0.70330	0.71738	0.97576	2c
	c=4.866	H3 0.99344	0.72295	0.68680	2c
	α= 90	H4 0.70290	0.28592	0.68713	2c
	β=119.3788	H5 0.29140	0.22593	0.98690	2c

	γ=90	H6 0.00296 0.22539 0.27370	2c
		H13 0.13461 -0.00000 0.62136	1a
		H14 0.03989 -0.00000 0.93453	1a
		H15 0.64392 -0.00000 0.11900	1a
		H16 0.94809 -0.00000 0.01841	1a
		H17 0.74420 -0.00000 0.52941	1a
		H18 0.54718 -0.00000 0.73103	1a
		H19 0.26233 0.50000 0.43775	1b
		H20 0.94450 0.50000 0.89729	1b
		H21 0.84486 0.50000 0.29908	1b
		H22 0.05816 0.50000 0.06766	1b
		H23 0.30801 0.50000 0.82379	1b
		H24 0.45162 0.50000 0.23376	1b
		Ru1 0.66593 0.25011 0.31299	2c
		Ru2 0.33027 0.74996 0.64878	2c
Imma-OsH_6	a=7.9047	H1 0.36766 1.03443 0.34801	16j
100 GPa	b=5.3247	H9 0.50000 0.81936 0.47210	8h
	c=4.7549	H10 -0.00000 0.58267 0.69928	8h
	α=β=γ=90	H17 -0.10493 0.75000 0.32278	8i
		H21 0.20685 1.25000 0.03547	8i
		Ru1 0.17097 0.50000 0.50000	8f

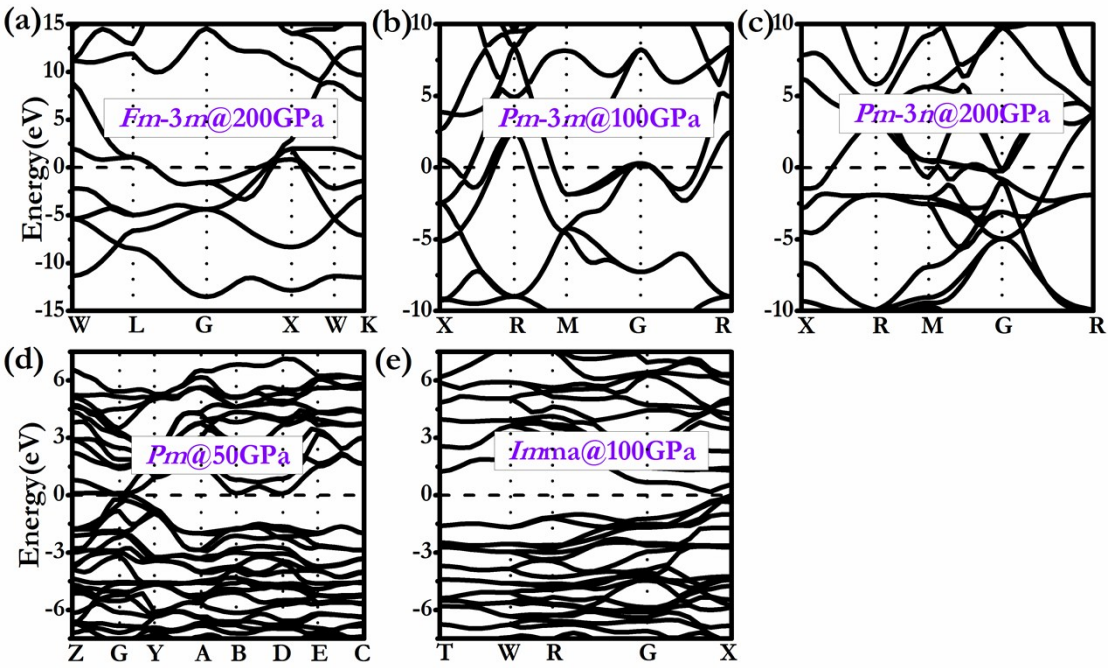

Fig. S1. The electronic band structures of the $Fm\bar{3}m$ (RuH), $Pm\bar{3}m$ (RuH_3), $Pm\bar{3}n$ (RuH_3), *Pm* (RuH_6) and *Imma* (RuH_6) at 200, 100, 200, 50, 100 GPa, respectively.

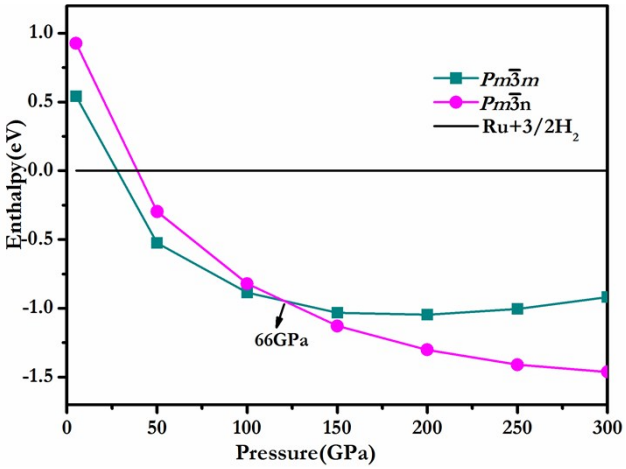

Fig. S2. Enthalpy curves (relative to Ru and H_2) for RuH_3 in the pressure range from 0 to 300 GPa.

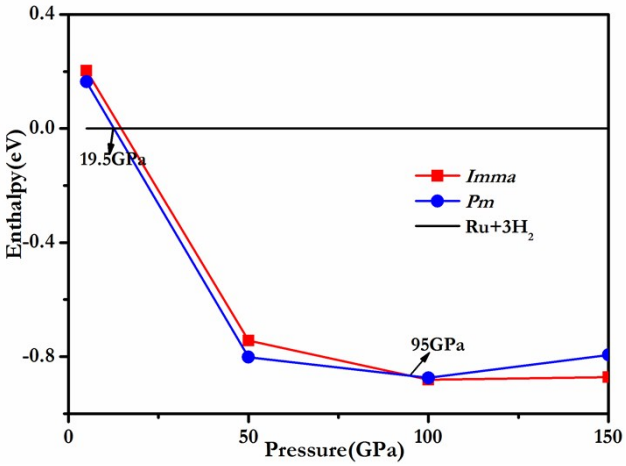

Fig. S3. Enthalpy curves (relative to Ru and H_2) for RuH_6 in the pressure range from 5 to 150 GPa.