

Supplementary Information

Enhancement of T_c in atomic phase of iodine-doped hydrogen at high pressures

Defang Duan, Fubo Tian, Yunxian Liu, Xiaoli Huang, Da Li, Hongyu Yu, Yanbin

*Ma, Bingbing Liu, Tian Cui**

*State Key Laboratory of Superhard Materials, College of Physics,
Jilin University, Changchun 130012, People's Republic of China*

*Electronic address: cuitian@jlu.edu.cn

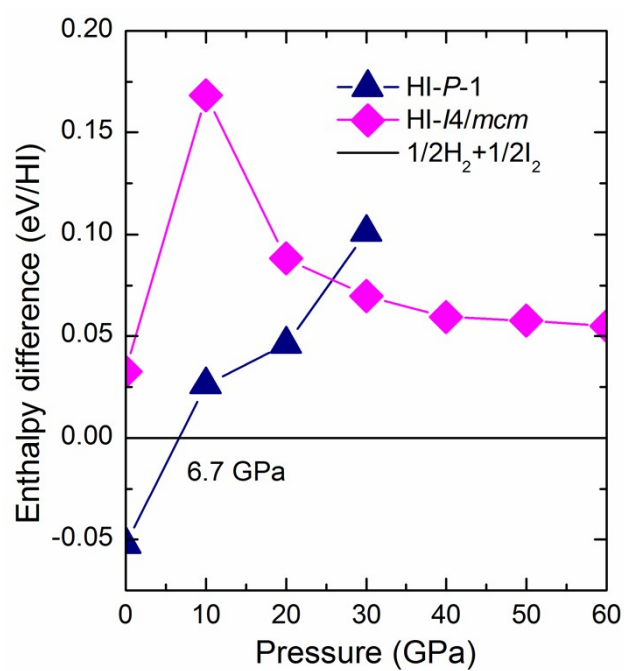


Fig. S1 The calculated enthalpy differences of *P*-1 and *I4/mcm* phases in HI with respect to decomposition into constituent elemental solids H₂ and I₂ as a function of pressure.

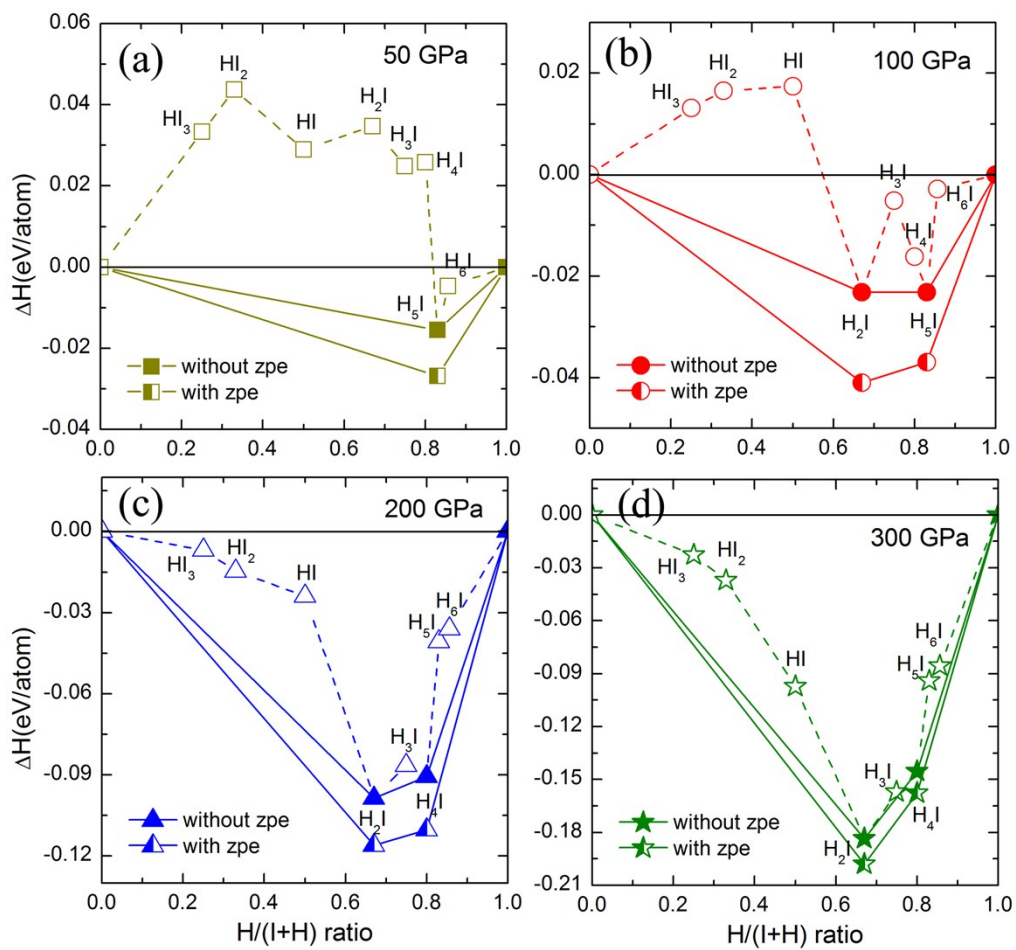


Fig. S2. Formation enthalpies of H-I system with respect to decomposition into constituent elemental solids under pressure. Dashed lines connect data points, and solid lines denote the convex hull. Solid and half-filled symbols indicate formation enthalpies of stable structures without and with ZPE, respectively.

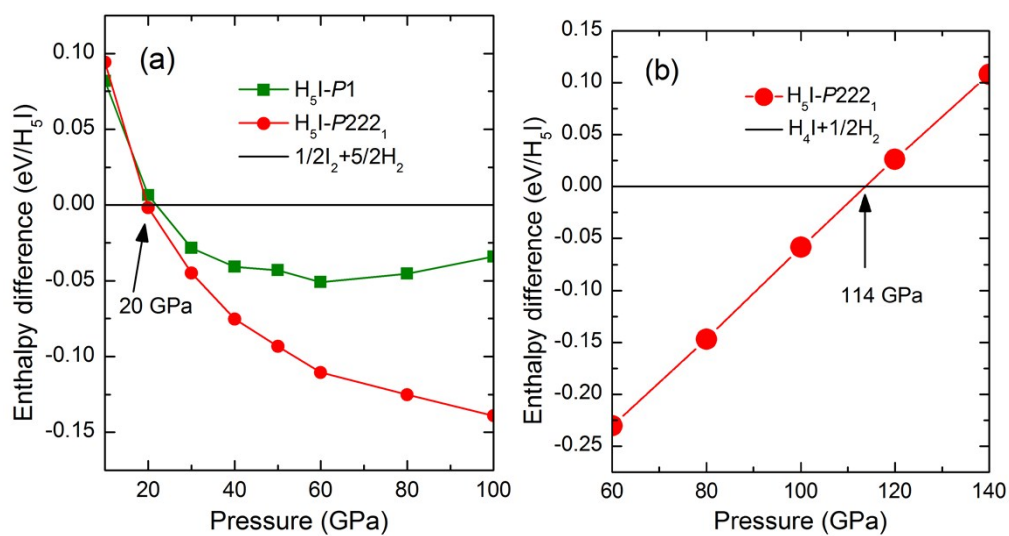


Fig. S3 (a) The calculated enthalpies of formation as a function of pressure for predicted H_5I . (b) The calculated enthalpy differences of $H_5I-P222_1$ phase with respect to decomposition into H_2 and H_4I as a function of pressure.

Table S1 Structure parameters of H and I atoms for our predicted stable structures of H-I compounds at the selected pressure.

Space group	Lattice parameters (Å, °)	Atom	Atomic coordinates (fractional)		
			x	y	z
H ₂ I- <i>Pmna</i> (200 GPa)	<i>a</i> =5.847	H(8d)	-0.03489	0.40070	0.87921
	<i>b</i> =2.727	I(4c)	0.17825	0.75000	0.62030
	<i>c</i> =4.389				
H ₂ I- <i>R-3m</i> (260 GPa)	<i>a</i> =3.056	H(6c)	0.00000	0.00000	0.40676
	<i>b</i> =5.897	I(3a)	0.00000	0.000000	0.00000
H ₄ I- <i>P6/mmm</i> (200 GPa)	<i>a</i> =2.996	H(4h)	0.33333	0.66667	0.34832
	<i>b</i> =2.669	I(1a)	0.00000	0.00000	0.00000
H ₃ I- <i>P222</i> ₁ (100 GPa)	<i>a</i> =6.553 <i>b</i> =3.178 <i>c</i> =5.524	H(4e)	0.44116	0.77691	0.08234
		H(4e)	0.04076	0.19417	0.93730
		H(4e)	0.55080	0.71453	0.08797
		H(4e)	0.03438	0.34861	0.61381
		H(2d)	0.50000	0.72936	0.75000
		H(2b)	0.24729	0.50000	-0.00000
		I(4e)	0.76196	0.21098	0.23417