Electronic Supplementary Information for

”Assessment of Density Functional Theory to Calculate Phase Transition Pressure of Ice”

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Table S1. Comparison table between the phase transition pressures in Gpa obtained from the intersection point of enthalpy and those from internal energy with equation (1).

Functional	Obtained from	Ih → II	Ih → III	II → VI	VI → VII	III → VI	Ih → VII	II → VII	III → VII
BLYP	Intersection point of Enthalpy	1.71	1.22	1.74	--	2.70	2.72	--	--
	Internal energy (EL + Ezpt) with eq. (1)	1.70	1.21	1,66	--	2.66	2.66	4.07	4.56
B3LYP	Intersection point of Enthalpy	1.23	0.93	1.35	--	2.03	2.35	--	--
	Internal energy (EL + Ezpt) with eq. (1)	1.22	0.97	1.31	--	1.89	2.27	3.88	--
PBE0	Intersection point of Enthalpy	1.18	0.92	1.37	--	1.94	2.24	--	--
	Internal energy (EL + Ezpt) with eq. (1)	1.18	0.93	1.31	--	1.85	--	3.72	3.83
	Exp.	0.014 ± 0.02	0.24 ± 0.01	1.05 ± 0.1	2 ± 0.1				

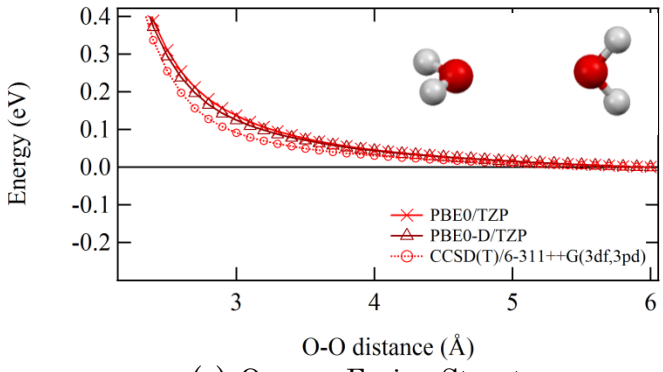
Table S2. Calculated phase transition pressures in GPa at various functionals whose experimental values were not reported previously.

	Zero point	III → VI	Ih → VII	II → VII	III → VII
BLYP	w/o	2.07	2.75	4.10	4.03
BLYP	with	2.13	2.72		
PW91	w/o	2.13	2.65	3.65	3.60
PBE	w/o	1.91	2.49	3.54	3.46
PBE-D	w/o	-0.36	0.11	-0.07	-0.01
PBEsol	w/o	1.50	2.13	2.61	2.62
B3LYP	w/o	3.36	2.48	3.64	4.24
B3LYP	with	2.03	2.35		
PBE0	w/o	4.40	2.36	3.19	4.06
PBE0	with	1.94	2.24		
PBE0-D	w/o	0.77	0.12	-0.17	0.15

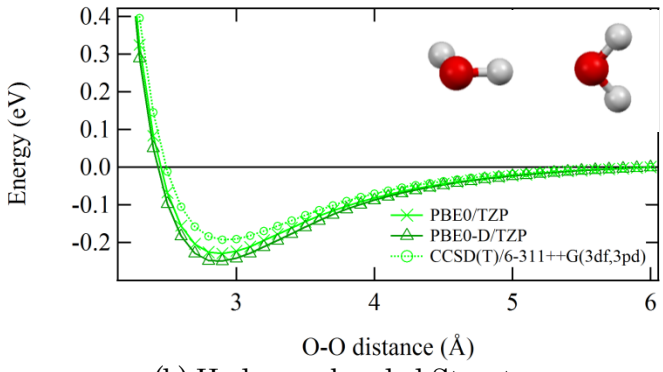
Table S3. Calculated phase transition pressures at PBE0 functional in various scaling factors whose experimental values were not reported. Units are in GPa.

	s_6	III → VI	Ih → VII	II → VII	III → VII
PBE0-D		4.40	2.36	3.19	4.05
	0.25	2.73	1.60	2.06	2.51
	0.50	1.33	0.85	0.93	1.33
	0.75	0.77	0.12	-0.17	0.15
	1.00	-0.03	-0.59	-1.35	-0.09

Figure S1 Energies of water dimer in different conformation. (a) oxygen facing structure, (b) hydrogen bonded structure. Solid lines with cross mark, triangle and circles are results by PBE0/TZP, PBE0/TZP (CRYSTAL09), and CCSD(T)/6-311++G(3df,3dp) (Gaussian 09), respectively. All the data are shifted by setting the energies at the O-O length of 6.0 Å to zero.



(a) Oxygen Facing Structure



(b) Hydrogen bonded Structure