SUPPORTING INFORMATION

New metallic ice phase under high pressure

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Table S1. Fractional coordinates of the TiO_2_brookite-*Pbca* structure with orthorhombic lattice (space group: *Pbca*; lattice constants: a = 5.436 Å, b = 2.669 Å, c = 2.669 Å) at *P* = 1000 GPa.

Atom	*X*	*Y*	*Z*	Occupancy
O	0.37463	0.50095	0.74083	1.0
H	0.02268	0.29685	0.69590	1.0
H	0.27737	0.44203	0.43927	1.0

Table S2. Fractional coordinates of the NaO_2-*Pa*3 structure with cubic lattice (space group: *Pa*3; lattice constants: a = b = c = 2.451 Å) at pressure of 2000 GPa.

Atom	*X*	*Y*	*Z*	Occupancy
O	0.0	0.0	0.0	1.0
H	0.36404	0.36404	0.36404	1.0

Table S3. Band gap (in eV) based on PBE functionals for Ag_2O-$Pn\bar{3}m$, TiO_2_brookite-*Pbca* and NaO_2-*Pa*3 phases. For the NaO_2-*Pa*3 structure, the band gap calculated using HSE06 hybrid functional is also provided in parentheses.

Pressure (GPa)	Band gap (eV)

	Ag_2O- $Pn\bar{3}m$	TiO_2_brookite-*Pbca*	NaO_2-*Pa*3
500	9.4122		
1000	8.1659	4.9993	1.2502 (2.6275)
1500	7.1088	2.8780	0.7760 (2.0816)
2000	6.1535	1.5859	0.3901 (1.6153)
2500	5.2825	0.8891	0.0919 (1.2844)
3000			0 (1.0285)
4000			0 (0.6883)
5000			0 (0.4991)
6000			0 (0.2895)
7000			0 (0.2337)

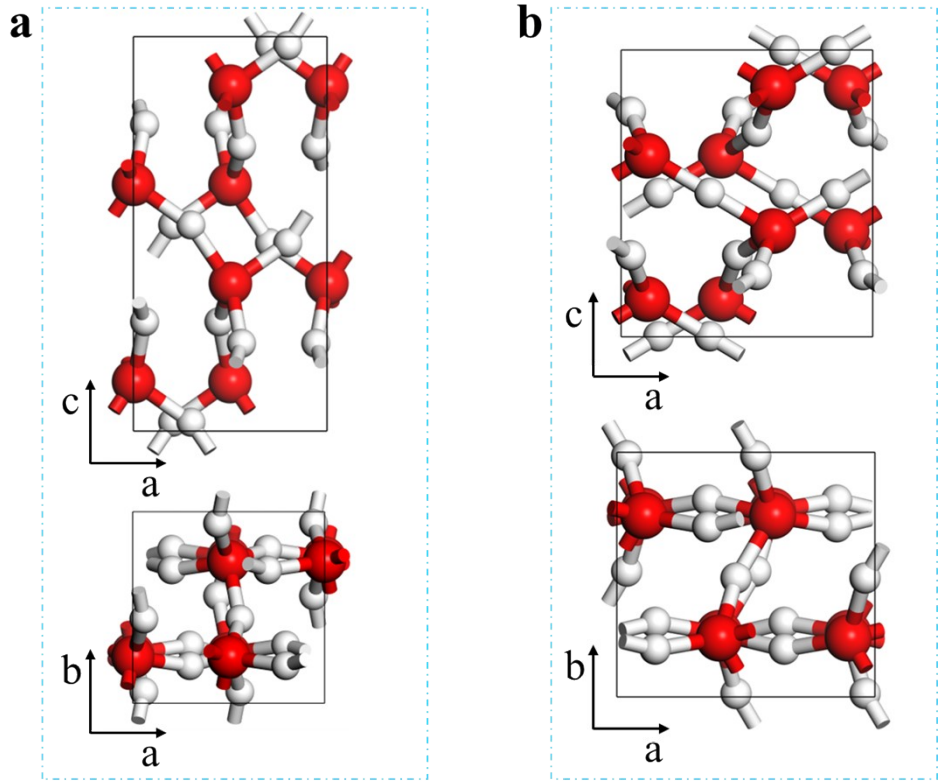

Figure S1. Crystal structures. (a) TiO_2_brookite-*Pbca* structure at pressure of 1000 GPa in this work. (b) *Pbca* phase at pressure of 1000 GPa from Ref. [1]. The large red spheres and small white spheres denote the O and H atoms, respectively.

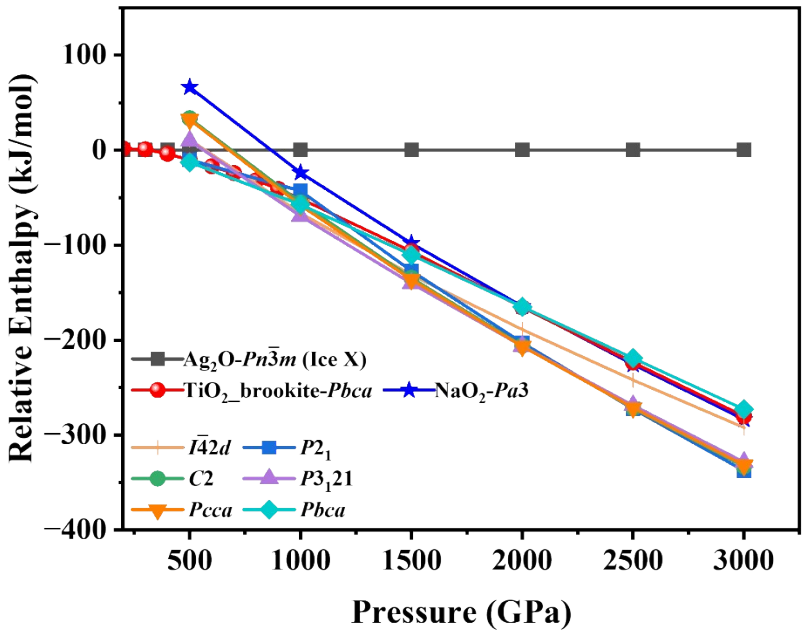

Figure S2. Relative enthalpy per water molecule versus pressure for ice phases, with Ag_2O-$Pn\bar{3}m$ (ice X) as a reference. The high-pressure phases of $I\bar{4}2d$, $P2_1$, $C2$, $P3_121$, *Pcca* and *Pbca* are from Ref. [1] and Ref. [2].

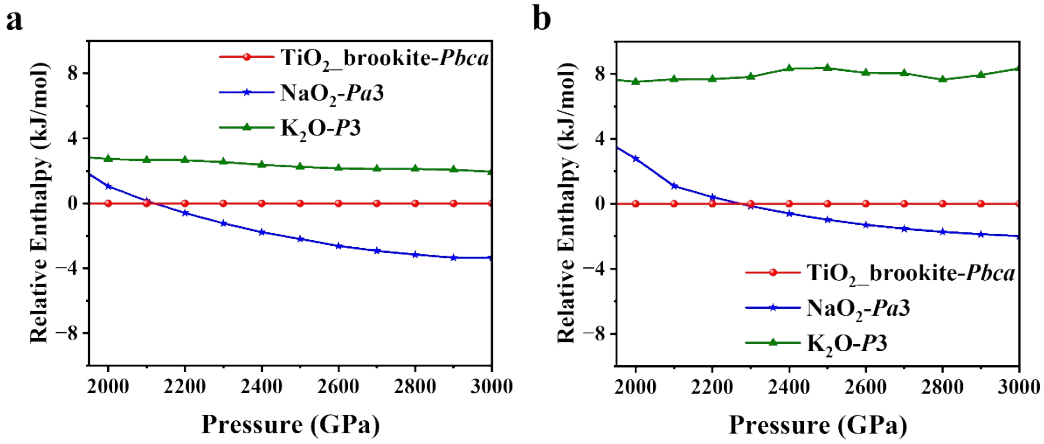

Figure S3. Relative enthalpy of ice phase at the pressure around 2000 to 3000 GPa, with TiO_2_brookite-*Pbca* as a reference. (a) Old relative enthalpy per water molecule versus pressure for ice phases based on soft PAW pseudopotentials. (b) New relative enthalpy per water molecule versus pressure for ice phases with hard PAW pseudopotentials and zero-point energy.

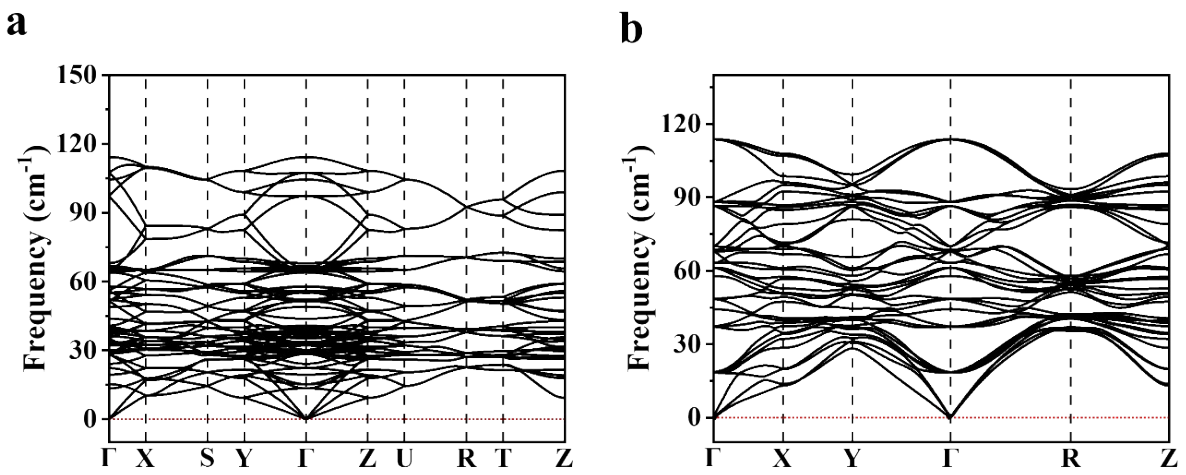

Figure S4. Phonon spectrum for (a) TiO_2_brookite-*Pbca* at P = 300 GPa and (b) NaO_2-*Pa*3 at P = 2200 GPa.

References

1. Y. Wang, H. Liu, J. Lv, L. Zhu, H. Wang and Y. Ma, *Nat. Commun.* 2011, **2**, 563.
2. C. J. Pickard, M. Martinez-Canales and R. J. Needs, *Phys. Rev. Lett.* 2013, **110**, 245701.
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