

## References

- [1] Brovchenko I, Oleinikova A. Multiple Phases of Liquid Water. *Chem Phys Chem* 2008; 9: 2660–2675. <https://doi.org/10.1002%2Fcpch.200800639>
- [2] Kepler J. *The six-cornered snowflake*. Oxford: Oxford University Press, 2014.
- [3] Ball P. In retrospect: On the Six-Cornered Snowflake. *Nature* 2011; 480: 455–455. <https://doi.org/10.1038%2F480455a>
- [4] Ludwig R, Paschek D. Wasser: Anomalien und Rätsel. *Chem Unserer Zeit* 2005; 39: 455-455. <https://doi.org/10.1038%2F480455a>
- [5] Cavendish H. Three Papers, Containing Experiments on Factitious Air, by the Hon. Henry Cavendish, F. R. S. *Philos Trans R Soc Lond* 1766; 56: 141–184. <https://doi.org/10.1098%2Frstl.1766.0019>
- [6] Priestley J, Hey W. Observations on Different Kinds of Air. *Philos Trans 1683-1775* 1772; 62: 147–264. <http://www.jstor.org/stable/106051>
- [7] Tanaka M, Girard G, Davis R, Peuto A and N Bignell. Recommended table for the density of water between 0 °C and 40 °C based on recent experimental reports. *Metrologia* 2001; 38: 301. <http://stacks.iop.org/0026-1394/38/i=4/a=3>
- [8] Hahn R. The Experimenters. A Study of the Accademia del Cimento. *Science* 1972; 177: 983–983. <https://doi.org/10.1126%2Fscience.177.4053.983>
- [9] Chemical Rubber Company, Lide DR (eds). *CRC handbook of chemistry and physics: a ready-reference book of chemical and physical data*. 84th ed. Boca Raton: CRC Press, 2003.
- [10] Malkin T L, Murray B J, Brukhno A V, et al. Structure of ice crystallized from supercooled water. *Proc Natl Acad Sci* 2012; 109: 1041–1045. <https://doi.org/10.1073%2Fpnas.1113059109>
- [11] Kamb B. Ice. II. A proton-ordered form of ice. *Acta Crystallogr* 1964; 17: 1437–1449. <https://doi.org/10.1107%2F50365110X64003553>
- [12] Kamb B, Prakash A. Structure of ice III. *Acta Crystallogr B* 1968; 24: 1317–1327. <https://doi.org/10.1107%2F50567740868004231>
- [13] Engelhardt H, Kamb B. Structure of ice IV, a metastable high-pressure phase. *J Chem Phys* 1981; 75: 5887–5899. <https://doi.org/10.1063%2F1.442040>

- [14] Kamb B, Prakash A, Knobler C. Structure of ice V. *Acta Crystallogr* 1967; 22: 706–715. <https://doi.org/10.1107%2FS0365110X67001409>
- [15] Kamb B. Structure of Ice VI. *Science* 1965; 150: 205–209. <https://doi.org/10.1126%2Fscience.150.3693.205>
- [16] Kamb B, Davis BL. Ice VII, the densest form of ice. *Proc Natl Acad Sci* 1964; 52: 1433–1439. <http://www.ncbi.nlm.nih.gov/pmc/articles/PMC300465/>
- [17] Whalley E, Davidson D W, Heath J B R. Dielectric Properties of Ice VII. Ice VIII: A New Phase of Ice. *J Chem Phys* 1966; 45: 3976–3982. <https://doi.org/10.1063%2F1.1727447>
- [18] Whalley E, Heath JBR, Davidson DW. Ice IX: An Antiferroelectric Phase Related to Ice III. *J Chem Phys* 1968; 48: 2362–2370. <https://doi.org/10.1063%2F1.1669438>
- [19] Hirsch K., Holzapfel W. Symmetric hydrogen bonds in ice X. *Phys Lett A* 1984; 101: 142–144. [https://doi.org/10.1016%2F0375-9601\(84\)90510-3](https://doi.org/10.1016%2F0375-9601(84)90510-3)
- [20] Fukazawa H, Ikeda S, Mae S. Incoherent inelastic neutron scattering measurements on ice XI; the proton-ordered phase of ice Ih doped with KOH. *Chem Phys Lett* 1998; 282: 215–218. [https://doi.org/10.1016%2FS0009-2614\(97\)01266-9](https://doi.org/10.1016%2FS0009-2614(97)01266-9)
- [21] Lobban C, Finney J L, Kuhs W F. The structure of a new phase of ice. *Nature* 1998; 391: 268–270. <https://doi.org/10.1038%2F34622>
- [22] Salzmann C G, Radaelli P G, Hallbrucker A, et al. The Preparation and Structures of Hydrogen Ordered Phases of Ice. *Science* 2006; 311: 1758–1761. <https://doi.org/10.1126%2Fscience.1123896>
- [23] Salzmann C G, Radaelli P G, Mayer E, et al. Ice XV: A New Thermodynamically Stable Phase of Ice. *Phys Rev Lett* 2009; 103: 105701. <https://doi.org/10.1103%2FPhysRevLett.103.105701>
- [24] Falenty A, Hansen T C, Kuhs W F. Formation and properties of ice XVI obtained by emptying a type sII clathrate hydrate. *Nature* 2014; 516: 231–233. <https://doi.org/10.1038%2Fnature14014>
- [25] del Rosso L, Celli M, Ulivi L. New porous water ice metastable at atmospheric pressure obtained by emptying a hydrogen-filled ice. *Nat Commun* 2016; 7: 13394. <https://doi.org/10.1038%2Fncomms13394>
- [26] Mishima O, Calvert L D, Whalley E. ‘Melting ice’ I at 77 K and 10 kbar: a new method of making amorphous solids. *Nature* 1984; 310: 393–395. <https://doi.org/10.1038%2F310393a0>

- [27] Mishima O, Calvert L D, Whalley E. An apparently first-order transition between two amorphous phases of ice induced by pressure. *Nature* 1985; 314: 76–78.  
<https://doi.org/10.1038%2F314076a0>
- [28] Loerting T, Salzmann C, Kohl I, et al. A second distinct structural “state” of high-density amorphous ice at 77 K and 1 bar. *Phys Chem Chem Phys* 2001; 3: 5355–5357.  
<https://doi.org/10.1039%2Fb108676f>
- [29] Loerting T, Winkel K, Seidl M, et al. How many amorphous ices are there? *Phys Chem Chem Phys* 2011; 13: 8783–8794.  
<https://doi.org/10.1039%2Fc0cp02600j>
- [30] Debenedetti P G. Supercooled and glassy water. *J Phys Condens Matter* 2003; 15: R1669.  
<http://stacks.iop.org/0953-8984/15/i=45/a=R01>
- [31] Champagnon B, Martinet C, Coussa C, et al. Polyamorphism: Path to new high density glasses at ambient conditions. *J Non-Cryst Solids* 2007; 353: 4208–4211.  
<https://doi.org/10.1016%2Fj.jnoncrysol.2007.07.026>
- [32] McMillan P F, Wilson M, Daisenberger D, et al. A density-driven phase transition between semiconducting and metallic polyamorphs of silicon. *Nat Mater* 2005; 4: 680–684.  
<https://doi.org/10.1038%2Fnm1458>
- [33] Grimsditch M. Polymorphism in Amorphous SiO<sub>2</sub>. *Phys Rev Lett* 1984; 52: 2379–2381.  
<https://doi.org/10.1103%2FPhysRevLett.52.2379>
- [34] Saika-Voivod I, Poole P H, Sciortino F. Fragile-to-strong transition and polyamorphism in the energy landscape of liquid silica. *Nature* 2001; 412: 514–517.  
<https://doi.org/10.1038%2F35087524>
- [35] Majérus O, Cormier L, Itié J-P, et al. Pressure-induced Ge coordination change and polyamorphism in SiO<sub>2</sub>–GeO<sub>2</sub> glasses. *J Non-Cryst Solids* 2004; 345–346: 34–38.  
<https://doi.org/10.1016%2Fj.jnoncrysol.2004.07.039>
- [36] Greaves G N, Wilding M C, Langstaff D, et al. Composition and polyamorphism in supercooled yttria–alumina melts. *J Non-Cryst Solids* 2011; 357: 435–441.  
<https://doi.org/10.1016%2Fj.jnoncrysol.2010.06.072>
- [37] Weber J K R, Abadie J G, Hixson A D, et al. Glass Formation and Polyamorphism in Rare-Earth Oxide-Aluminum Oxide Compositions. *J Am Ceram Soc* 2004; 83: 1868–1872.  
<https://doi.org/10.1111%2Fj.1151-2916.2000.tb01483.x>
- [38] Wilding M C, McMillan P F. Polyamorphic transitions in yttria–alumina liquids. *J Non-Cryst Solids* 2001; 293–295: 357–365. [https://doi.org/10.1016%2FS0022-3093\(01\)00686-X](https://doi.org/10.1016%2FS0022-3093(01)00686-X)

- [39] Stillinger F H. Water Revisited. *Science* 1980; 209: 451–457.  
<https://doi.org/10.1126%2Fscience.209.4455.451>
- [40] Poole P H, Sciortino F, Grande T, et al. Effect of Hydrogen Bonds on the Thermodynamic Behavior of Liquid Water. *Phys Rev Lett* 1994; 73: 1632–1635.  
<https://doi.org/10.1103%2FPhysRevLett.73.1632>
- [41] Errington J R, Debenedetti P G. Relationship between structural order and the anomalies of liquid water. *Nature* 2001; 409: 318–321.  
<http://dx.doi.org/10.1038/35053024>
- [42] Stokely K, Mazza M G, Stanley H E, et al. Effect of hydrogen bond cooperativity on the behavior of water. *Proc Natl Acad Sci* 2010; 107: 1301–1306.  
<https://doi.org/10.1073%2Fpnas.0912756107>
- [43] Russo J, Tanaka H. Understanding water's anomalies with locally favoured structures. *Nat Commun* 2014; 5: 3556. <https://doi.org/10.1038%2Fncoms4556>
- [44] Suresh S J, Naik V M. Hydrogen bond thermodynamic properties of water from dielectric constant data. *J Chem Phys* 2000; 113: 9727–9732.  
<https://doi.org/10.1063%2F1.1320822>
- [45] Silverstein K A T, Haymet A D J, Dill K A. The Strength of Hydrogen Bonds in Liquid Water and Around Nonpolar Solutes. *J Am Chem Soc* 2000; 122: 8037–8041.  
<https://doi.org/10.1021%2Fja000459t>
- [46] Smith J D. Energetics of Hydrogen Bond Network Rearrangements in Liquid Water. *Science* 2004; 306: 851–853. <https://doi.org/10.1126%2Fscience.1102560>
- [47] Debenedetti P G. Supercooled and glassy water. *J Phys Condens Matter* 2003; 15: R1669.  
<http://stacks.iop.org/0953-8984/15/i=45/a=R01>
- [48] Gallo P, Amann-Winkel K, Angell C A, et al. Water: A Tale of Two Liquids. *Chem Rev* 2016; 116: 7463–7500. <https://doi.org/10.1021%2Facs.chemrev.5b00750>
- [49] Speedy R J. Stability-limit conjecture. An interpretation of the properties of water. *J Phys Chem* 1982; 86: 982–991. <https://doi.org/10.1021%2Fj100395a030>
- [50] Poole P H, Sciortino F, Essmann U, et al. Phase behaviour of metastable water. *Nature* 1992; 360: 324–328. <https://doi.org/10.1038%2F360324a0>
- [51] Sastry S, Debenedetti P G, Sciortino F, et al. Singularity-free interpretation of the thermodynamics of supercooled water. *Phys Rev E* 1996; 53: 6144–6154.  
<https://doi.org/10.1103%2FPhysRevE.53.6144>

- [52] Angell C A. Insights into Phases of Liquid Water from Study of Its Unusual Glass-Forming Properties. *Science* 2008; 319: 582–587.  
<https://doi.org/10.1126%2Fscience.1131939>
- [53] Amann-Winkel K, Böhmer R, Fujara F, et al. *Colloquium*: Water's controversial glass transitions. *Rev Mod Phys* 2016; 88: 011002.  
<https://doi.org/10.1103%2FRevModPhys.88.011002>
- [54] Bernal J D, Fowler R H. A Theory of Water and Ionic Solution, with Particular Reference to Hydrogen and Hydroxyl Ions. *J Chem Phys* 1933; 1: 515–548.  
<https://doi.org/10.1063%2F1.1749327>
- [55] Kuhs W F, Lehmann M S. The Structure of Ice-Ih. In: Franks F (ed) *Water Science Reviews* 2. Cambridge: Cambridge University Press, pp. 1–66.  
<http://ebooks.cambridge.org/ref/id/CBO9780511897504A005>
- [56] Walrafen G E. Raman Spectral Studies of Water Structure. *J Chem Phys* 1964; 40: 3249–3256. <https://doi.org/10.1063%2F1.1724992>
- [57] Fuentes-Landete V, Mitterdorfer C, Handle P H, et al. Crystalline and amorphous ices. *Proc Int Sch Phys Enrico Fermi* 2015; 173–208. <https://doi.org/10.3254%2F978-1-61499-507-4-173>
- [58] Singer S J, Kuo J-L, Hirsch T K, et al. Hydrogen-Bond Topology and the Ice VII / VIII and Ice I<sub>h</sub>/ XI Proton-Ordering Phase Transitions. *Phys Rev Lett* 2005; 94:135701.  
<https://doi.org/10.1103%2FPhysRevLett.94.135701>
- [59] Knight C, Singer S J, Kuo J-L, et al. Hydrogen bond topology and the ice VII/VIII and I<sub>h</sub>/XI proton ordering phase transitions. *Phys Rev E* 2006; 73:056113.  
<https://doi.org/10.1103%2FPhysRevE.73.056113>
- [60] Fan X, Bing D, Zhang J, et al. Predicting the hydrogen bond ordered structures of ice Ih, II, III, VI and ice VII: DFT methods with localized based set. *Comput Mater Sci* 2010; 49: S170–S175. <https://doi.org/10.1016%2Fj.commatsci.2010.04.004>
- [61] Fukazawa H, Ikeda S, Oguro M, et al. Deuteron Ordering in KOD-Doped Ice Observed by Neutron Diffraction. *J Phys Chem B* 2002; 106: 6021–6024.  
<https://doi.org/10.1021%2Fjp020688x>
- [62] Kuo J-L, Klein M L, Kuhs W F. The effect of proton disorder on the structure of ice-Ih: A theoretical study. *J Chem Phys* 2005; 123: 134505.  
<https://doi.org/10.1063%2F1.2036971>
- [63] Lobban C, Finney J L, Kuhs W F. The structure and ordering of ices III and V. *J Chem Phys* 2000; 112: 7169–7180. <https://doi.org/10.1063%2F1.481282>

- [64] La Placa S J, Hamilton W C, Kamb B, et al. On a nearly proton-ordered structure for ice IX. *J Chem Phys* 1973; 58: 567–580. <https://doi.org/10.1063%2F1.1679238>
- [65] Nishibata K, Whalley E. Thermal effects of the transformation ice III–IX. *J Chem Phys* 1974; 60: 3189–3194. <https://doi.org/10.1063%2F1.1681505>
- [66] Minčeva-Šukarova B, Shermann W F, Wilkinson G R. A high pressure spectroscopic study on the ice III — ice IX disordered — ordered transition. *J Mol Struct* 1984; 115: 137–140. [https://doi.org/10.1016%2F0022-2860\(84\)80033-2](https://doi.org/10.1016%2F0022-2860(84)80033-2)
- [67] Londono J D, Kuhs W F, Finney J L. Neutron diffraction studies of ices III and IX on under-pressure and recovered samples. *J Chem Phys* 1993; 98: 4878–4888. <https://doi.org/10.1063%2F1.464942>
- [68] Knight C, Singer S J. A reexamination of the ice III/IX hydrogen bond ordering phase transition. *J Chem Phys* 2006; 125: 064506. <https://doi.org/10.1063%2F1.2209230>
- [69] Salzmann C G, Hallbrucker A, Finney J L, et al. Raman spectroscopic study of hydrogen ordered ice XIII and of its reversible phase transition to disordered ice V. *Phys Chem Chem Phys* 2006; 8: 3088–3093. <https://doi.org/10.1039%2Fb604360g>
- [70] Salzmann C G, Radaelli P G, Finney J L, et al. A calorimetric study on the low temperature dynamics of doped ice V and its reversible phase transition to hydrogen ordered ice XIII. *Phys Chem Chem Phys* 2008; 10: 6313–6324. <https://doi.org/10.1039%2Fb808386j>
- [71] Knight C, Singer S J. Hydrogen bond ordering in ice V and the transition to ice XIII. *J Chem Phys* 2008; 129: 164513. <https://doi.org/10.1063%2F1.2991297>
- [72] Kuhs W F, Finney J L, Vettier C, et al. Structure and hydrogen ordering in ices VI, VII, and VIII by neutron powder diffraction. *J Chem Phys* 1984; 81: 3612–3623. <https://doi.org/10.1063%2F1.448109>
- [73] Knight C, Singer S J. Prediction of a Phase Transition to a Hydrogen Bond Ordered Form of Ice VI. *J Phys Chem B* 2005; 109: 21040–21046. <https://doi.org/10.1021%2Fjp0540609>
- [74] Kuo J-L, Kuhs W F. A First Principles Study on the Structure of Ice-VI: Static Distortion, Molecular Geometry, and Proton Ordering. *J Phys Chem B* 2006; 110: 3697–3703. <https://doi.org/10.1021%2Fjp055260n>
- [75] Jorgensen J D, Beyerlein R A, Watanabe N, et al. Structure of D<sub>2</sub>O ice VIII from *in situ* powder neutron diffraction. *J Chem Phys* 1984; 81: 3211–3214. <https://doi.org/10.1063%2F1.448027>
- [76] Jorgensen J D, Worlton T G. Disordered structure of D<sub>2</sub>O ice VII from *in situ* neutron powder diffraction. *J Chem Phys* 1985; 83: 329–333. <https://doi.org/10.1063%2F1.449867>

- [77] Pruzan P, Chervin J D and M. Gauthier. Raman Spectroscopy Investigation of Ice VII and Deuterated Ice VII to 40 GPa. Disorder in Ice VII. *EPL Europhys Lett* 1990; 13: 81. <http://stacks.iop.org/0295-5075/13/i=1/a=014>
- [78] Pruzan P, Chervin J C, Canny B. Determination of the D<sub>2</sub>O ice VII–VIII transition line by Raman scattering up to 51 GPa. *J Chem Phys* 1992; 97: 718–721. <https://doi.org/10.1063%2F1.463570>
- [79] Besson J M, Pruzan P, Klotz S, et al. Variation of interatomic distances in ice VIII to 10 GPa. *Phys Rev B* 1994; 49: 12540–12550. <https://doi.org/10.1103%2FPhysRevB.49.12540>
- [80] Besson J M, Kobayashi M, Nakai T, et al. Pressure dependence of Raman linewidths in ices VII and VIII. *Phys Rev B* 1997; 55: 11191–11201. <https://doi.org/10.1103%2FPhysRevB.55.11191>
- [81] Pruzan P, Chervin J C, Wolanin E, et al. Phase diagram of ice in the VII–VIII–X domain. Vibrational and structural data for strongly compressed ice VIII. *J Raman Spectrosc* 2003; 34: 591–610. <https://doi.org/10.1002%2Fjrs.1039>
- [82] Song M, Yamawaki H, Fujihisa H, et al. Infrared investigation on ice VIII and the phase diagram of dense ices. *Phys Rev B* 2003; 68:014106. <https://doi.org/10.1103%2FPhysRevB.68.014106>
- [83] Yoshimura Y, Stewart S T, Somayazulu M, et al. High-pressure x-ray diffraction and Raman spectroscopy of ice VIII. *J Chem Phys* 2006; 124: 024502. <https://doi.org/10.1063%2F1.2140277>
- [84] Somayazulu M, Shu J, Zha C, et al. *In situ* high-pressure x-ray diffraction study of H<sub>2</sub>O ice VII. *J Chem Phys* 2008; 128: 064510. <https://doi.org/10.1063%2F1.2813890>
- [85] Salzmann C G, Hallbrucker A, Finney J L, et al. Raman spectroscopic features of hydrogen-ordering in ice XII. *Chem Phys Lett* 2006; 429: 469–473. <https://doi.org/10.1016%2Fj.cplett.2006.08.079>
- [86] Tribello G A, Slater B, Salzmann C G. A Blind Structure Prediction of Ice XIV. *J Am Chem Soc* 2006; 128: 12594–12595. <https://doi.org/10.1021%2Fja0630902>
- [87] Martin-Conde M, MacDowell L G, Vega C. Computer simulation of two new solid phases of water: Ice XIII and ice XIV. *J Chem Phys* 2006; 125: 116101. <https://doi.org/10.1063%2F1.2354150>
- [88] Noya E G, Conde M M, Vega C. Computing the free energy of molecular solids by the Einstein molecule approach: Ices XIII and XIV, hard-dumbbells and a patchy model of proteins. *J Chem Phys* 2008; 129: 104704. <https://doi.org/10.1063%2F1.2971188>

- [89] Kuhs W F, Lehmann M S. The structure of the ice Ih by neutron diffraction. *J Phys Chem* 1983; 87: 4312–4313. <https://doi.org/10.1021%2Fj100244a063>
- [90] Moore E B, Molinero V. Is it cubic? Ice crystallization from deeply supercooled water. *Phys Chem Chem Phys* 2011; 13: 20008. <https://doi.org/10.1039%2F0c1cp22022e>
- [91] Malkin T L, Murray B J, Salzmann C G, et al. Stacking disorder in ice I. *Phys Chem Chem Phys* 2015; 17: 60–76. <https://doi.org/10.1039%2FC4CP02893G>
- [92] Kuhs W F, Sippel C, Falenty A, et al. Extent and relevance of stacking disorder in ‘ice Ic’. *Proc Natl Acad Sci* 2012; 109: 21259–21264. <https://doi.org/10.1073%2Fpnas.1210331110>
- [93] Petrenko VvF, Whitworth RvW. *Physics of ice*. Oxford; New York: Oxford University Press, 1999.
- [94] König H. Eine kubische Eismodifikation. *ZKristallogr* 1943; 105: 279–86.
- [95] Hansen T C, Koza M M, Kuhs W F. Formation and annealing of cubic ice: I. Modelling of stacking faults. *J Phys Condens Matter* 2008; 20: 285104. <https://doi.org/10.1088%2F0953-8984%2F20%2F28%2F285104>
- [96] Hansen T C, Koza M M, Lindner P, et al. Formation and annealing of cubic ice: II. Kinetic study. *J Phys Condens Matter* 2008; 20: 285105. <https://doi.org/10.1088%2F0953-8984%2F20%2F28%2F285105>
- [97] Bauer M, Elsaesser M S, Winkel K, et al. Compression-rate dependence of the phase transition from hexagonal ice to ice II and/or ice III. *Phys Rev B* 2008; 77:220105. <https://doi.org/10.1103%2FPhysRevB.77.220105>
- [98] Bauer M, Winkel K, Toebbens D M, et al. Hexagonal ice transforms at high pressures and compression rates directly into “doubly metastable” ice phases. *J Chem Phys* 2009; 131: 224514. <https://doi.org/10.1063%2F1.3271651>
- [99] Wilson G J, Chan R K, Davidson D W, et al. Dielectric Properties of Ices II, III, V, and VI. *J Chem Phys* 1965; 43: 2384–2391. <https://doi.org/10.1063%2F1.1697137>
- [100] Fortes A D, Wood I G, Brodholt J P, et al. *Ab initio* simulation of the ice II structure. *J Chem Phys* 2003; 119: 4567–4572. <https://doi.org/10.1063%2F1.1593630>
- [101] Seidl M, Fayter A, Stern JN, et al. Shrinking water’s no man’s land by lifting its low-temperature boundary. *Phys Rev B* 2015; 91: 144201. <https://doi.org/10.1103%2FPhysRevB.91.144201>
- [102] Burton E F, Oliver W F. X-Ray Diffraction Patterns of Ice. *Nature* 1935; 135: 505–506. <https://doi.org/10.1038%2F135505b0>



- [103] Brüggeller P, Mayer E. Complete vitrification in pure liquid water and dilute aqueous solutions. *Nature* 1980; 288: 569–571. <https://doi.org/10.1038%2F288569a0>
- [104] Mayer E, Brüggeller P. Vitrification of pure liquid water by high pressure jet freezing. *Nature* 1982; 298: 715–718. <https://doi.org/10.1038%2F298715a0>
- [105] Mayer E. New method for vitrifying water and other liquids by rapid cooling of their aerosols. *J Appl Phys* 1985; 58: 663–667. <https://doi.org/10.1063%2F1.336179>
- [106] Winkel K, Bowron D T, Loerting T, et al. Relaxation effects in low density amorphous ice: Two distinct structural states observed by neutron diffraction. *J Chem Phys* 2009; 130: 204502. <https://doi.org/10.1063%2F1.3139007>
- [107] Winkel K, Elsaesser M S, Mayer E, et al. Water polyamorphism: Reversibility and (dis) continuity. *J Chem Phys* 2008; 128: 044510. <https://doi.org/10.1063%2F1.2830029>
- [108] Winkel K, Bauer M, Mayer E, et al. Structural transitions in amorphous H<sub>2</sub>O and D<sub>2</sub>O: the effect of temperature. *J Phys Condens Matter* 2008; 20: 494212. <https://doi.org/10.1088%2F0953-8984%2F20%2F49%2F494212>
- [109] Bowron D T, Finney J L, Hallbrucker A, et al. The local and intermediate range structures of the five amorphous ices at 80K and ambient pressure: A Faber-Ziman and Bhatia-Thornton analysis. *J Chem Phys* 2006; 125: 194502. <https://doi.org/10.1063%2F1.2378921>
- [110] Seidl M, Amann-Winkel K, Handle PH, et al. From parallel to single crystallization kinetics in high-density amorphous ice. *Phys Rev B* 2013; 88: 174105. <https://doi.org/10.1103%2FPhysRevB.88.174105>
- [111] Tse JS. Mechanical instability in ice  $I_h$ . A mechanism for pressure-induced amorphization. *J Chem Phys* 1992; 96: 5482–5487. <https://doi.org/10.1063%2F1.462732>
- [112] Strässle T, Saitta A M, Klotz S, et al. Phonon Dispersion of Ice under Pressure. *Phys Rev Lett* 2004; 93: 225901. <https://doi.org/10.1103%2FPhysRevLett.93.225901>
- [113] Mishima O. Relationship between melting and amorphization of ice. *Nature* 1996; 384: 546–549. <https://doi.org/10.1038%2F384546a0>
- [114] Tse J S, Klug D D, Tulk C A, et al. The mechanisms for pressure-induced amorphization of ice  $I_h$ . *Nature* 1999; 400: 647–649. <https://doi.org/10.1038%2F23216>
- [115] Strässle T, Klotz S, Hamel G, et al. Experimental Evidence for a Crossover between Two Distinct Mechanisms of Amorphization in Ice  $I_h$  under Pressure. *Phys Rev Lett* 2007; 99: 175501. <https://doi.org/10.1103%2FPhysRevLett.99.175501>

- [116] Strässle T, Caviezel A, Padmanabhan B, et al. Temperature dependence of the pressure-induced amorphization of ice Ih studied by high-pressure neutron diffraction to 30 K. *Phys Rev B* 2010; 82: 094103. <https://doi.org/10.1103%2FPhysRevB.82.094103>
- [117] Nelmes R J, Loveday J S, Strässle T, et al. Annealed high-density amorphous ice under pressure. *Nat Phys* 2006; 2: 414–418. <https://doi.org/10.1038%2Fnpphys313>
- [118] Winkel K, Mayer E, Loerting T. Equilibrated High-Density Amorphous Ice and Its First-Order Transition to the Low-Density Form. *J Phys Chem B* 2011; 115: 14141–14148. <https://doi.org/10.1021%2Fjp203985w>
- [119] Loerting T, Giovambattista N. Amorphous ices: experiments and numerical simulations. *J Phys Condens Matter* 2006; 18: R919–R977. <https://doi.org/10.1088%2F0953-8984%2F18%2F50%2FR01>
- [120] Loerting T, Schustereder W, Winkel K, et al. Amorphous Ice: Stepwise Formation of Very-High-Density Amorphous Ice from Low-Density Amorphous Ice at 125 K. *Phys Rev Lett* 2006; 96: 025702. <https://doi.org/10.1103%2FPhysRevLett.96.025702>
- [121] Wedler G, Freund H-J. *Lehrbuch der physikalischen Chemie*. Sechste, vollständig überarbeitete und aktualisierte Auflage. Weinheim: Wiley-VCH Verlag GmbH & Co. KGaA, 2012.
- [122] Bovenkamp P. Phasenübergang im frühen Universum. <https://www.uni-muenster.de/Physik.TP/archive/fileadmin/lehre/teilchen/ws1112/Phasenuebergaenge.pdf>
- [123] Dieterich W. Theorie der Phasenübergänge, Fachbereich Physik, Universität Konstanz. [http://theorie.physik.uni-konstanz.de/dieterich/skripte/Theorie-der-Phasenuebergaenge\\_Skript.pdf](http://theorie.physik.uni-konstanz.de/dieterich/skripte/Theorie-der-Phasenuebergaenge_Skript.pdf)
- [124] Püschl W. Phasenübergänge in Festkörpern, Phänomenologie und Thermodynamik, Skriptum zu einer Vorlesung im Wintersemester 2010, Fakultät für Physik, Universität Wien. [https://www.univie.ac.at/physikwiki/images/4/48/Skript\\_Phasen%20C3%BCberg%20C-3%A4ngeWS10.pdf](https://www.univie.ac.at/physikwiki/images/4/48/Skript_Phasen%20C3%BCberg%20C-3%A4ngeWS10.pdf)
- [125] Debenedetti P G. *Metastable liquids: concepts and principles*. Princeton, N.J: Princeton University Press, 1996.
- [126] Stöckel P. *Homogene Nukleation in levitierten Tröpfchen aus stark unterkühltem H<sub>2</sub>O und D<sub>2</sub>O*. Digitale Dissertation, FU Berlin. <http://webdoc.sub.gwdg.de/ebook/diss/2003/fu-berlin/2002/23/> (2002).
- [127] Fanfoni M, Tomellini M. The Johnson-Mehl- Avrami-Kohnogorov model: A brief review. *Il Nuovo Cimento D* 1998; 20: 1171–1182. <https://doi.org/10.1007%2FBBF03185527>

- [128] Avrami M. Kinetics of Phase Change. I General Theory. *J Chem Phys* 1939; 7: 1103–1112. <https://doi.org/10.1063%2F1.1750380>
- [129] Avrami M. Kinetics of Phase Change. II Transformation-Time Relations for Random Distribution of Nuclei. *J Chem Phys* 1940; 8: 212–224. <https://doi.org/10.1063%2F1.1750631>
- [130] Avrami M. Granulation, Phase Change, and Microstructure Kinetics of Phase Change. III. *J Chem Phys* 1941; 9: 177–184. <https://doi.org/10.1063%2F1.1750872>
- [131] Mishima O. Reversible first-order transition between two H<sub>2</sub>O amorphs at ~0.2 GPa and ~135 K. *J Chem Phys* 1994; 100: 5910–5912. <https://doi.org/10.1063%2F1.467103>
- [132] Loerting T, Brazhkin V V, Morishita T. Multiple Amorphous–Amorphous Transitions. In: Rice SA (ed) *Advances in Chemical Physics*. Hoboken, NJ, USA: John Wiley & Sons, Inc., pp. 29–82. <http://doi.wiley.com/10.1002/9780470508602.ch2>
- [133] Yoshimura Y, Mao H and Hemley R J. In Situ Raman spectroscopy of reversible low-temperature transition between low-density and high-density amorphous ices. *J Phys Condens Matter* 2007; 19: 425214. <http://stacks.iop.org/0953-8984/19/i=42/a=425214>
- [134] Klotz S, Strässle T, Nelmes R J, et al. Nature of the Polyamorphic Transition in Ice under Pressure. *Phys Rev Lett* 2005; 94: 025506. <https://doi.org/10.1103%2FPhysRevLett.94.025506>
- [135] Mishima O, Takemura K, Aoki K. Visual Observations of the Amorphous-Amorphous Transition in H<sub>2</sub>O Under Pressure. *Science* 1991; 254: 406–408. <https://doi.org/10.1126%2Fscience.254.5030.406>
- [136] Tse J S, Klug D D, Guthrie M, et al. Investigation of the intermediate- and high-density forms of amorphous ice by molecular dynamics calculations and diffraction experiments. *Phys Rev B* 2005; 71: 214107. <https://doi.org/10.1103%2FPhysRevB.71.214107>
- [137] Guthrie M, Urquidi J, Tulk C A, et al. Direct structural measurements of relaxation processes during transformations in amorphous ice. *Phys Rev B* 2003; 68: 184110. <https://doi.org/10.1103%2FPhysRevB.68.184110>
- [138] Angell C A. Liquid Fragility and the Glass Transition in Water and Aqueous Solutions. *Chem Rev* 2002; 102: 2627–2650. <https://doi.org/10.1021%2Fcr000689q>
- [139] Menzel A. Skriptum zur Vorlesung ‘Feste Körper’ WS 2015/16.
- [140] Giovambattista N, Loerting T, Lukanov B R, et al. Interplay of the Glass Transition and the Liquid-Liquid Phase Transition in Water. *Sci Rep* 2012; 2: 390. <https://doi.org/10.1038%2Fspringer00390>

- [141] Johari G P, Hallbrucker A, Mayer E. The glass–liquid transition of hyperquenched water. *Nature* 1987; 330: 552–553. <https://doi.org/10.1038%2F330552a0>
- [142] Kohl I, Bachmann L, Mayer E, et al. Water Behaviour: Glass transition in hyperquenched water? *Nature* 2005; 435: E1–E1. <https://doi.org/10.1038%2Fnature03707>
- [143] Kohl I, Bachmann L, Hallbrucker A, et al. Liquid-like relaxation in hyperquenched water at  $\leq 140$  K. *Phys Chem Chem Phys* 2005; 7: 3210. <https://doi.org/10.1039%2Fb507651j>
- [144] Elsaesser M S, Winkel K, Mayer E, et al. Reversibility and isotope effect of the calorimetric glass  $\rightarrow$  liquid transition of low-density amorphous ice. *Phys Chem Chem Phys* 2010; 12: 708–712. <https://doi.org/10.1039%2FB917662D>
- [145] Mishima O. The glass-to-liquid transition of the emulsified high-density amorphous ice made by pressure-induced amorphization. *J Chem Phys* 2004; 121: 3161–3164. <https://doi.org/10.1063%2F1.1774151>
- [146] Andersson O. Relaxation Time of Water’s High-Density Amorphous Ice Phase. *Phys Rev Lett* 2005; 95: 205503. <https://doi.org/10.1103%2FPhysRevLett.95.205503>
- [147] Andersson O, Inaba A. Dielectric properties of high-density amorphous ice under pressure. *Phys Rev B* 2006; 74: 184201. <https://doi.org/10.1103%2FPhysRevB.74.184201>
- [148] Andersson O. Dielectric relaxation of the amorphous ices. *J Phys Condens Matter* 2008; 20: 244115. <https://doi.org/10.1088%2F0953-8984%2F20%2F24%2F244115>
- [149] Seidl M, Elsaesser MS, Winkel K, et al. Volumetric study consistent with a glass-to-liquid transition in amorphous ices under pressure. *Phys Rev B* 2011; 83: 100201(R). <https://doi.org/10.1103%2FPhysRevB.83.100201>
- [150] Andersson O. Glass-liquid transition of water at high pressure. *Proc Natl Acad Sci* 2011; 108: 11013–11016. <https://doi.org/10.1073%2Fpnas.1016520108>
- [151] Handle P H, Seidl M, Loerting T. Relaxation Time of High-Density Amorphous Ice. *Phys Rev Lett* 2012; 108: 225901. <https://doi.org/10.1103%2FPhysRevLett.108.225901>
- [152] Amann-Winkel K, Gainaru C, Handle P H, et al. Water’s second glass transition. *Proc Natl Acad Sci* 2013; 110: 17720–17725. <https://doi.org/10.1073%2Fpnas.1311718110>
- [153] Loerting T, Fuentes-Landete V, Handle P H, et al. The glass transition in high-density amorphous ice. *J Non-Cryst Solids* 2015; 407: 423–430. <https://doi.org/10.1016%2Fj.jnoncrsol.2014.09.003>

- [154] Handle P H, Loerting T. Dynamics anomaly in high-density amorphous ice between 0.7 and 1.1 GPa. *Phys Rev B* 2016; 93: 064204. <https://doi.org/10.1103%2FPhysRevB.93.064204>
- [155] Hill C R, Mitterdorfer C, Youngs T G A, et al. Neutron Scattering Analysis of Water's Glass Transition and Micropore Collapse in Amorphous Solid Water. *Phys Rev Lett* 2016; 116: 215501. <https://doi.org/10.1103%2FPhysRevLett.116.215501>
- [156] Perakis F, Amann-Winkel K, Lehmkuhler F, et al. Diffusive dynamics during the high-to-low density transition in amorphous ice. *Proc Natl Acad Sci* 2017; 114: 8193–8198. <https://doi.org/10.1073%2Fpnas.1705303114>
- [157] Pallares G, El Mekki Azouzi M, Gonzalez M A, et al. Anomalies in bulk supercooled water at negative pressure. *Proc Natl Acad Sci* 2014; 111: 7936–7941. <https://doi.org/10.1073%2Fpnas.1323366111>
- [158] Stanley H E, Kumar P, Xu L, et al. The puzzling unsolved mysteries of liquid water: Some recent progress. *Phys Stat Mech Its Appl* 2007; 386: 729–743. <https://doi.org/10.1016%2Fj.physa.2007.07.044>
- [159] Holten V, Qiu C, Guillemin E, et al. Compressibility Anomalies in Stretched Water and Their Interplay with Density Anomalies. *J Phys Chem Lett* 2017; 8: 5519–5522. <https://doi.org/10.1021%2Facs.jpclett.7b02563>
- [160] Mishima O, Stanley HE. Decompression-induced melting of ice IV and the liquid–liquid transition in water. *Nature* 1998; 392: 164–168. <https://doi.org/10.1038%2F32386>
- [161] González M A, Valeriani C, Caupin F, et al. A comprehensive scenario of the thermodynamic anomalies of water using the TIP4P/2005 model. *J Chem Phys* 2016; 145: 054505. <https://doi.org/10.1063%2F1.4960185>
- [162] Fuentevilla D A, Anisimov M A. Scaled Equation of State for Supercooled Water near the Liquid-Liquid Critical Point. *Phys Rev Lett* 2006; 97: 195702. <https://doi.org/10.1103%2FPhysRevLett.97.195702>
- [163] Mishima O. Volume of supercooled water under pressure and the liquid-liquid critical point. *J Chem Phys* 2010; 133: 144503. <https://doi.org/10.1063%2F1.3487999>
- [164] Holten V, Bertrand C E, Anisimov M A, et al. Thermodynamics of supercooled water. *J Chem Phys* 2012; 136: 094507. <https://doi.org/10.1063%2F1.3690497>
- [165] Stern J, Loerting T. Crystallisation of the amorphous ices in the intermediate pressure regime. *Sci Rep* 2017; 7. <https://doi.org/10.1038%2Fs41598-017-03583-2>
- [166] Seidl M, Fayter A, Stern J N, et al. High-performance dilatometry under extreme conditions. *Proceedings of the 6th Zwick Academia Day 2015*.

- [167] Tonauer C M, Seidl-Nigsch M, Loerting T. High-density amorphous ice: nucleation of nanosized low-density amorphous ice. *J Phys Condens Matter* 2018; 30: 034002. <https://doi.org/10.1088%2F1361-648X%2Faa9e76>
- [168] Massa W. *Kristallstrukturbestimmung*. 7., aktualisierte Aufl. Wiesbaden: Vieweg + Teubner, 2011.
- [169] Kunze-Liebhäuser J. Vorlesung ‘Grenzflächen - und Materialanalytik’ SS 2015.
- [170] Salzmann C G, Loerting T, Klotz S, et al. Isobaric annealing of high-density amorphous ice between 0.3 and 1.9 GPa: in situ density values and structural changes. *Phys Chem Chem Phys* 2006; 8: 386–397. <https://doi.org/10.1039%2Fb510168a>
- [171] Loerting T, Bauer M, Kohl I, et al. Cryoflotation: Densities of Amorphous and Crystalline Ices. *J Phys Chem B* 2011; 115: 14167–14175. <https://doi.org/10.1021%2Fjp204752w>
- [172] Hobbs PV. *Ice physics*. Oxford: Clarendon Press, 1974.
- [173] Whalley E, Klug D D, Handa Y P. Entropy of amorphous ice. *Nature* 1989; 342: 782–783. <https://doi.org/10.1038%2F342782a0>
- [174] Espinosa J R, Vega C, Sanz E. Ice–Water Interfacial Free Energy for the TIP4P, TIP4P/2005, TIP4P/Ice, and mW Models As Obtained from the Mold Integration Technique. *J Phys Chem C* 2016; 120: 8068–8075. <https://doi.org/10.1021%2Facs.jpcc.5b11221>
- [175] IAPWS. *Revised Release on Surface Tension of Ordinary Water Substance*. Moscow, 2014.
- [176] Vega C, de Miguel E. Surface tension of the most popular models of water by using the test-area simulation method. *J Chem Phys* 2007; 126: 154707. <https://doi.org/10.1063%2F1.2715577>
- [177] Russo J, Romano F, Tanaka H. New metastable form of ice and its role in the homogeneous crystallization of water. *Nat Mater* 2014; 13: 733–739. <https://doi.org/10.1038%2Fnmnat3977>
- [178] Fisher M, Devlin J P. Defect activity in amorphous ice from isotopic exchange data: insight into the glass transition. *J Phys Chem* 1995; 99: 11584–11590. <https://doi.org/10.1021%2Fj100029a041>
- [179] Shephard J J, Salzmann C G. Molecular Reorientation Dynamics Govern the Glass Transitions of the Amorphous Ices. *J Phys Chem Lett* 2016; 7: 2281–2285. <https://doi.org/10.1021%2Facs.jpclett.6b00881>