Review of: "Direct observation of ultrafast hydrogen bond strengthening in liquid water"

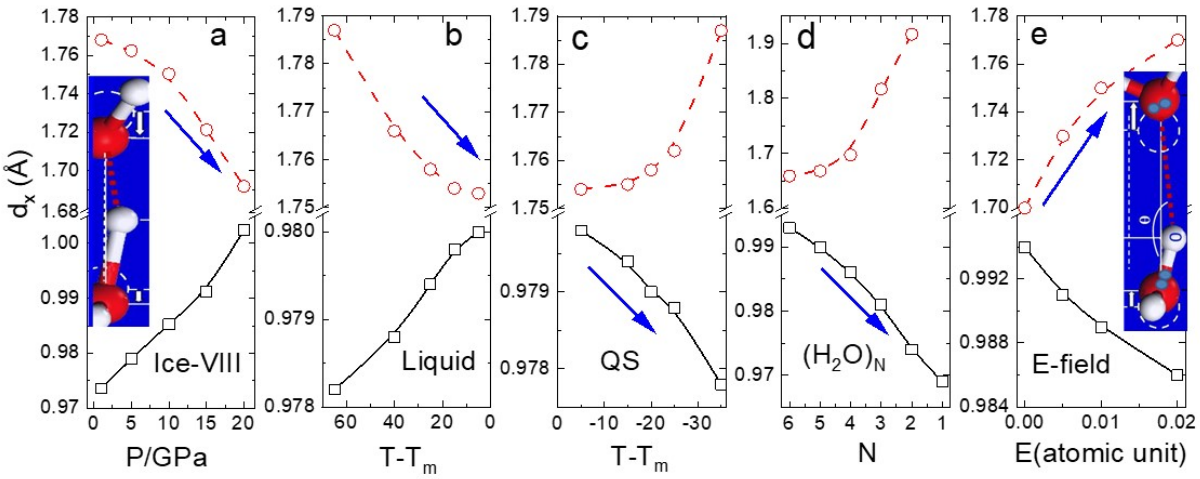
Changqing Sun[1]

1 Nanyang Technological University

Potential competing interests: The author(s) declared that no potential competing interests exist.

Sophisticated work [1] unveiled that the H–O bond contracts by 0.04 Å on a timescale of 80 femtosecond under 3,315 cm^{-1} infrared laser pulse in the 100 nm sized liquid droplet.

The H–O length change should be in the same frequency of the radiating laser source and associated with O:H elongation, according to the premise of hydrogen bond cooperativity and polarizability (HBCP) [2, 3]. The pressure, temperature, electric vector of the laser pulses, and the intrinsic molecular undercoordination in the skin shell of the droplet, serve as sources of perturbation. The a.c. polarization could be the factor dominating the a.c.H-O bond relaxation in the present case.



O—O repulsive coupling of the inter- and intramolecular interaction enabled O:H−O bond cooperativity and polarizability (HBCP): *ab initio* force field computation revealed the following: **a** Mechanical compression and **b** Liquid cooling shorten and stiffen the weaker O:H nonbond while do the stronger H−O bond contrastingly (subscript x = H−O, O:H in the vertical axis label); however, **c** Quasisolid

(QS) cooling, **d** molecular undercoordination, and **e** electrostatic polarization do the contrast, associated with strong polarization. The O:H−O relaxes in a “master-slave” manner and the H−O relaxes always less than the O:H in the same direction. Arrows denote the relaxation directions of the master segments.

1. Yang, J., R. Dettori, J.P.F. Nunes, N.H. List, E. Biasin, M. Centurion, Z. Chen, A.A. Cordones, D.P. Deponte, T.F. Heinz, M.E. Kozina, K. Ledbetter, M.-F. Lin, A.M. Lindenberg, M. Mo, A. Nilsson, X. Shen, T.J.A. Wolf, D. Donadio, K.J. Gaffney, T.J. Martinez, and X. Wang, *Direct observation of ultrafast hydrogen bond strengthening in liquid water.* Nature, 2021. **596**(7873): p. 531-535.
2. Sun, C.Q., *Water electrification: Principles and applications.* Adv. Coll. Interf. Sci., 2020. **282**: p. 102188.
3. Sun, C.Q., *Rules essential for water molecular undercoordination.* Chin. Phys. B, 2020. **8**(8): p. 088203.