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Ab initio theory of hydrogen-bond network in liquid water

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Water is of the utmost importance for life and technology. However, an accurate and genuinely predictive model of water has eluded scientists. We demonstrate that a fully ab initio approach, relying on the strongly constrained and appropriately normed (SCAN) density functional, provides such a description of water. SCAN accurately describes the balance among covalent bonds, hydrogen bonds, and van der Waals interactions that dictate the structure and dynamics of liquid water. Notably, SCAN captures the density difference between water and ice Ih at ambient conditions, as well as many important characteristics of the nuclear and electronic structures and dynamics of the liquid. These successful predictions of the versatile SCAN functional open the gates to study complex processes in aqueous phase chemistry and the interactions of water with other materials in an efficient, accurate, and completely predictive, ab initio manner.