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Structural dynamics of solvated OH^- and H_3O^+ in liquid water: an *ab initio* molecular dynamics study using PBE0 hybrid functional with van der Waals' interaction LIXIN ZHENG, XIFAN WU, Temple Univ — The nature of solvation structure of hydroxide (OH^-) and hydronium (H_3O^+) solvated in liquid water is of fundamental interest, as it is the prerequisite to understand the autoprotolysis process, which is often a crucial step in chemical and biological activities. It has been revealed that the proton transfer (PT) process, especially in hydroxide case, is of great controversy and complexity compared to traditional textbook description. One major source of inaccuracy originates from the delocalization error and lack of dispersion force in the conventional adopted electron exchange correlation function in GGA functional leading to an over-structured H-bond (HB) structure. Now with state-of-the-art PBE0 hybrid density functional, and the inclusion of long-range van der Waals dispersion force, we are able to perform *ab initio* molecular dynamics with higher accuracy. Through the analysis of mean square displacement of ion, HB geometrical distribution and lifetime, and the strength change of HB, we are presenting a quantitatively accurate picture of proton transfer structural mechanism.

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