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Solvated Hydroxide and Hydronium in Water Studied by ab initio Molecular Dynamics Based on PBE0 Hybrid Functional with van der Waals Interaction LIXIN ZHENG, CHARLES SWARTZ, XIFAN WU, Temple Univ — The nature of the solvation structures of hydroxide (OH^-) and hydronium (H_3O^+) aqueous solutions is of fundamental interest. It is the prerequisite to understanding the mechanism of proton transfer (PT) through the autoprotolysis process in water. For a long time, ab initio calculations based on local or semi-local approximations have been used to study the solvated OH^- and H_3O^+ . Although successfully giving a qualitative description of the proton mechanism, the semi-local functional suffers from the delocalization error. In addition, the description of dispersion force is missing. To overcome the above errors, we perform ab initio molecular dynamics calculations in both solvated OH^- and H_3O^+ based on PBE0 hybrid density functional and include the vander Waals interactions. It is found that, compared to the semi-local functional, the proton transfer rate in solvated OH^- reduces due to the changes in the solvation structure.

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