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The Molecular Structural and Electronic Properties of Liquid Water by *ab initio* Molecular Dynamics Simulation Based on SCAN Density Functional[1] LIXIN ZHENG, ZHAORU SUN, XIFAN WU, Department of Physics, Temple University — We performed the *ab initio* molecular dynamics (AIMD) simulation of liquid water based on the recently developed SCAN meta-GGA functional. It is well-known that bulk water simulation at GGA-level DFT has several drawbacks including over-structured H-bond, and slow diffusivity etc. With SCAN functional, the intermediate range many-body van der Waals effect is captured with a more accurate description of covalent bond at the same time. Based on the above improved functional description, we found that the liquid water structure is also improved by a less over-structured H-bond structure and faster diffusive property towards the experimental direction. At the same time, the electronic property including the dipole moment and band gaps are also improved compared to GGA DFT. Our work shows that SCAN is a promising candidate for the *ab initio* simulation of liquid water in the future.

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