Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

The electronic properties of water simulated using a first-principles van der Waals density functional approach

Changming Fang[1]*, *Wun-Fan Li*[1], *Rik S. Koster*[1], *Jiří Klimeš*[2],

Alfons van Blaaderen[1], *Marijn A. van Huis*[1]

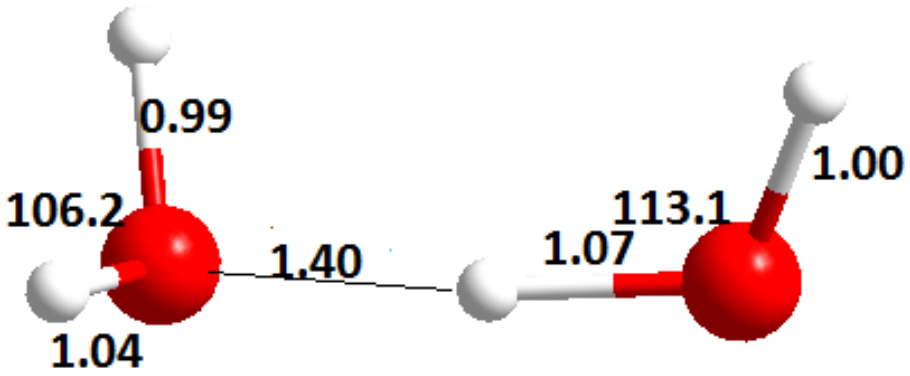
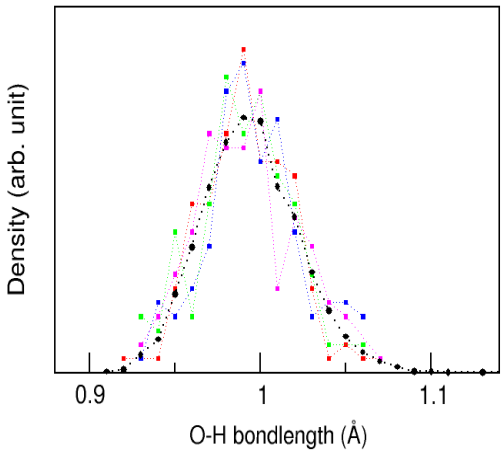


Figure S1. The schematic structure of a $(H_2O)_2$ cluster observed during the molecular dynamics simulations. The O—H bond has a long of about 1.4 Å while the other O–H bonds and the angles in the H2O molecules are varying with time.

a)



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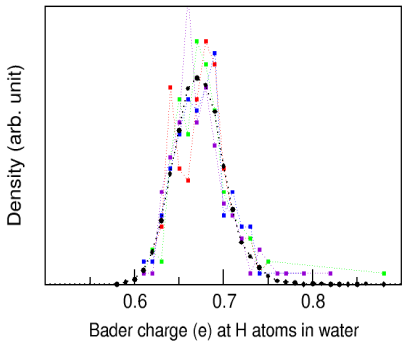

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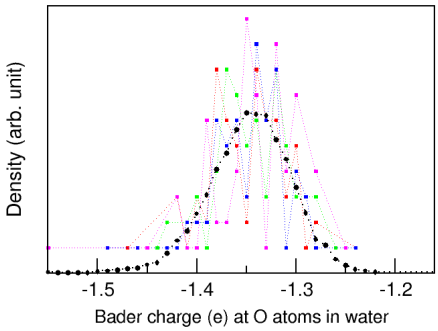

Figure S2. (a) Distributions for intra-molecular O-H bond-lengths, (b) Bader charges for H and (c) for O of four selected snapshots (colored in red, green, blue and magma) produced during the molecular dynamics simulations of water, and the time-averaged (black) at 300 K.

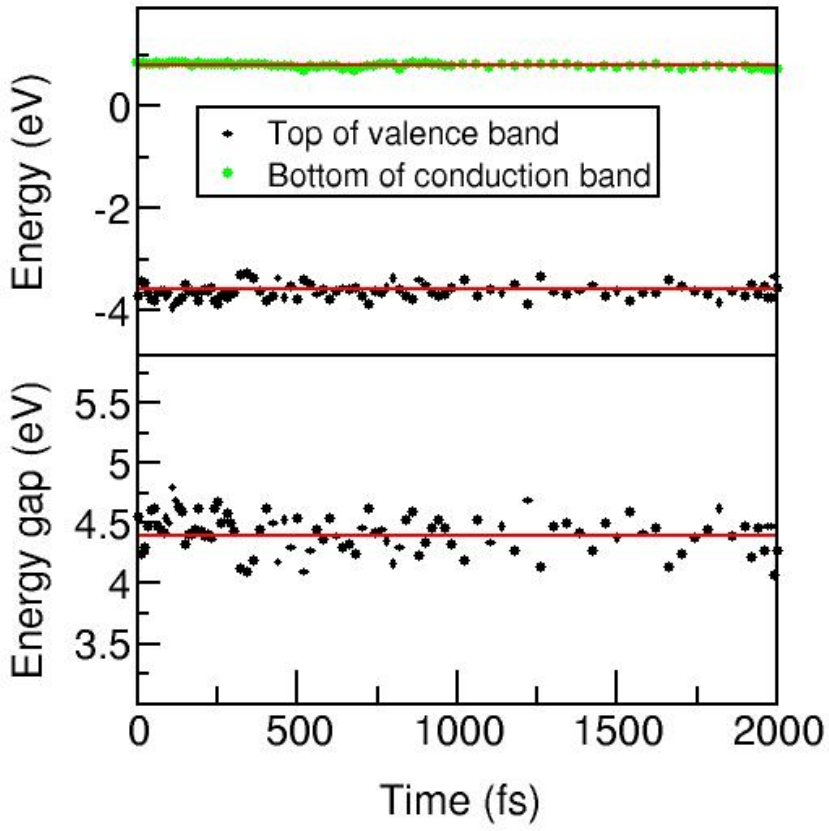

Figure S3. Dependences of highest occupied eigen-energy (black points, top), lowest unoccupied eigen-energy (green points, top) and energy gap (bottom, black circles) on time for water in 2ps.

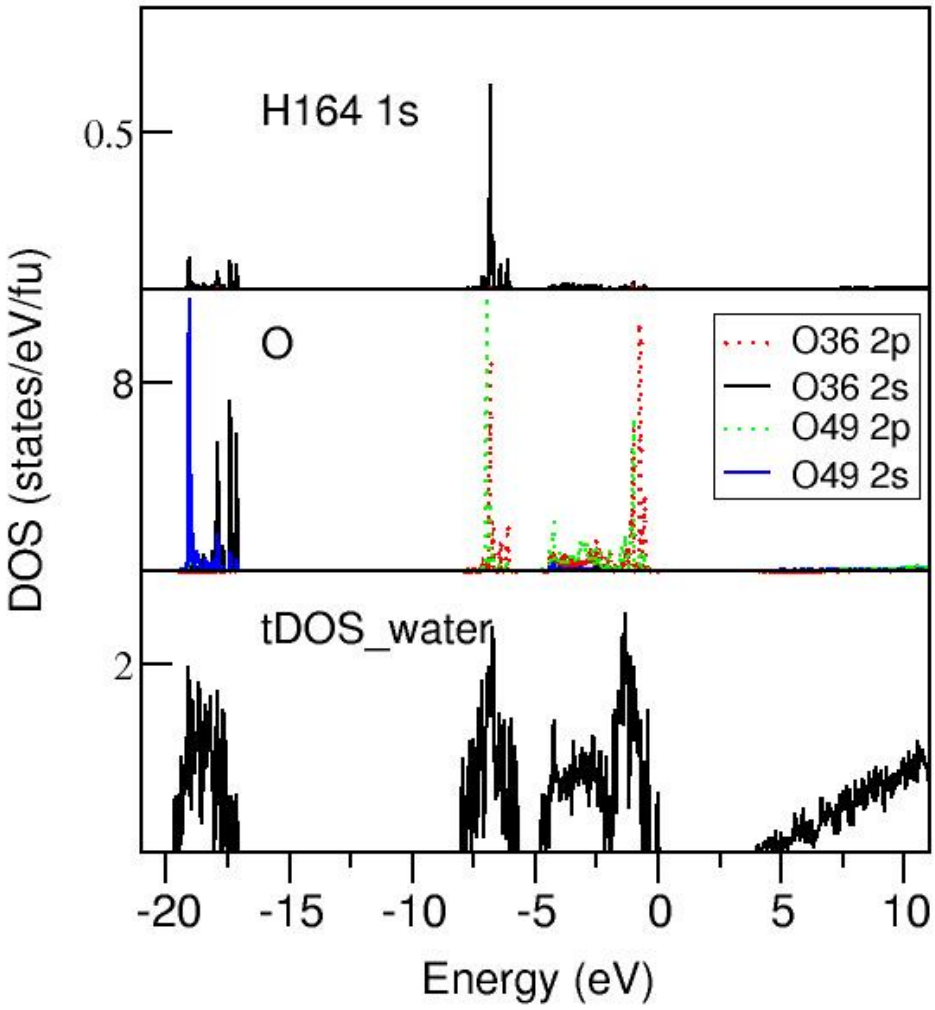

Figure S4: Partial DOS curves of the $2H_2O$ cluster (Figure S1) and the tDOS curve of the corresponding of water at simulated at 300 K.