Supporting information

Accurate SCC-DFTB parameterization for bulk water

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1. SCC-DFTB Radial Distribution Function of bulk water.

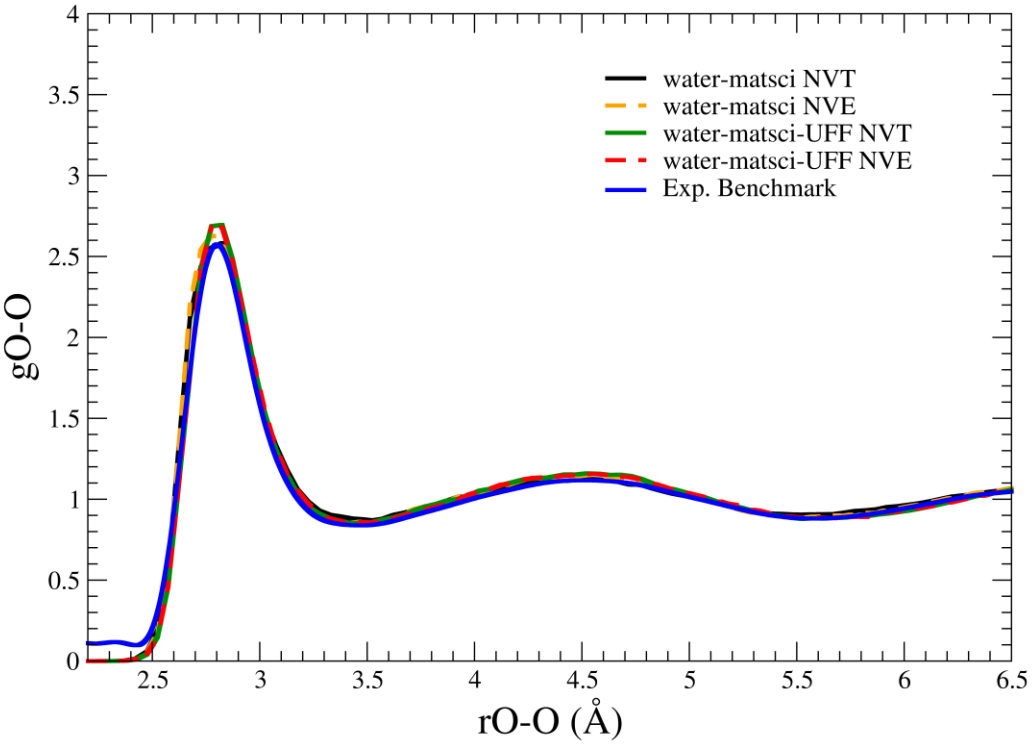


Figure S1. Radial distribution function for O-O obtained by IBI. NVT and NVE SCC-DFTB molecular dynamics by the water-matsci and water-matsci-UFF new parameters are shown.

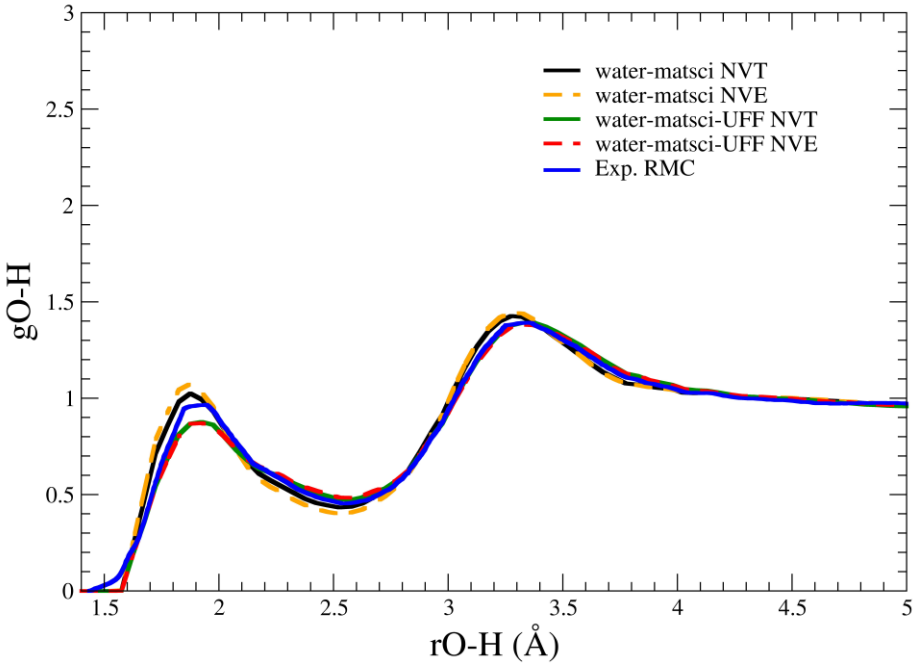


Figure S2. Radial distribution function for O-H obtained by IBI. NVT and NVE SCC-DFTB molecular dynamics by the water-matsci and water-matsci-UFF new parameters are shown.

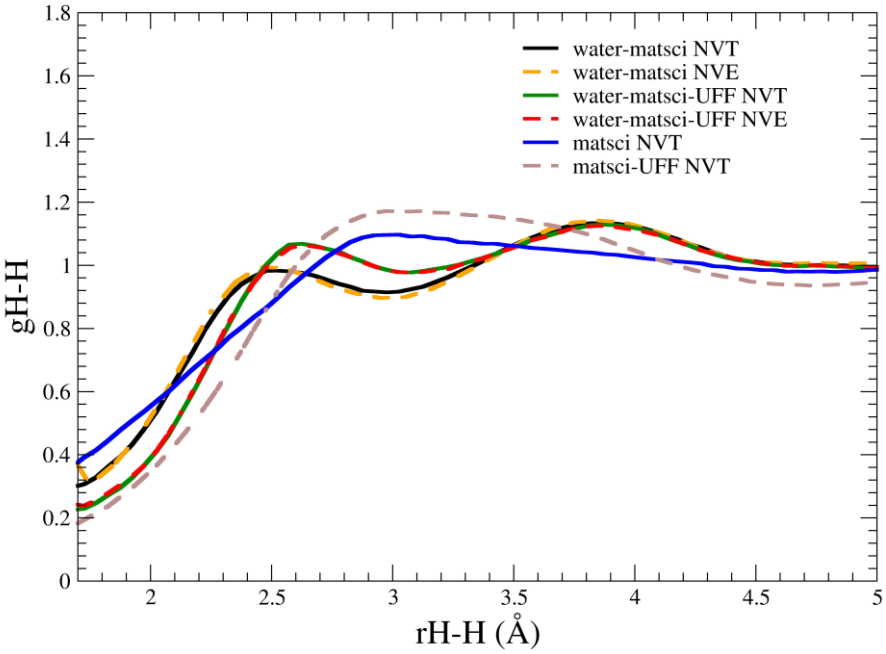


Figure S3. Radial distribution function for H-H obtained by IBI. NVT and NVE SCC-DFTB molecular dynamics by the water-matsci and water-matsci-UFF new parameters are shown.

2. Water neutralization reaction

Table S1- Neutralization energy (ΔH) for the different SCC-DFTB parameters. Values in kJ/mol.

Method	*ΔH*
water-matsci	***-193***
water-matsci-UFF	***-216***
matsci-UFF	***-262***
mio-UFF	***-188***

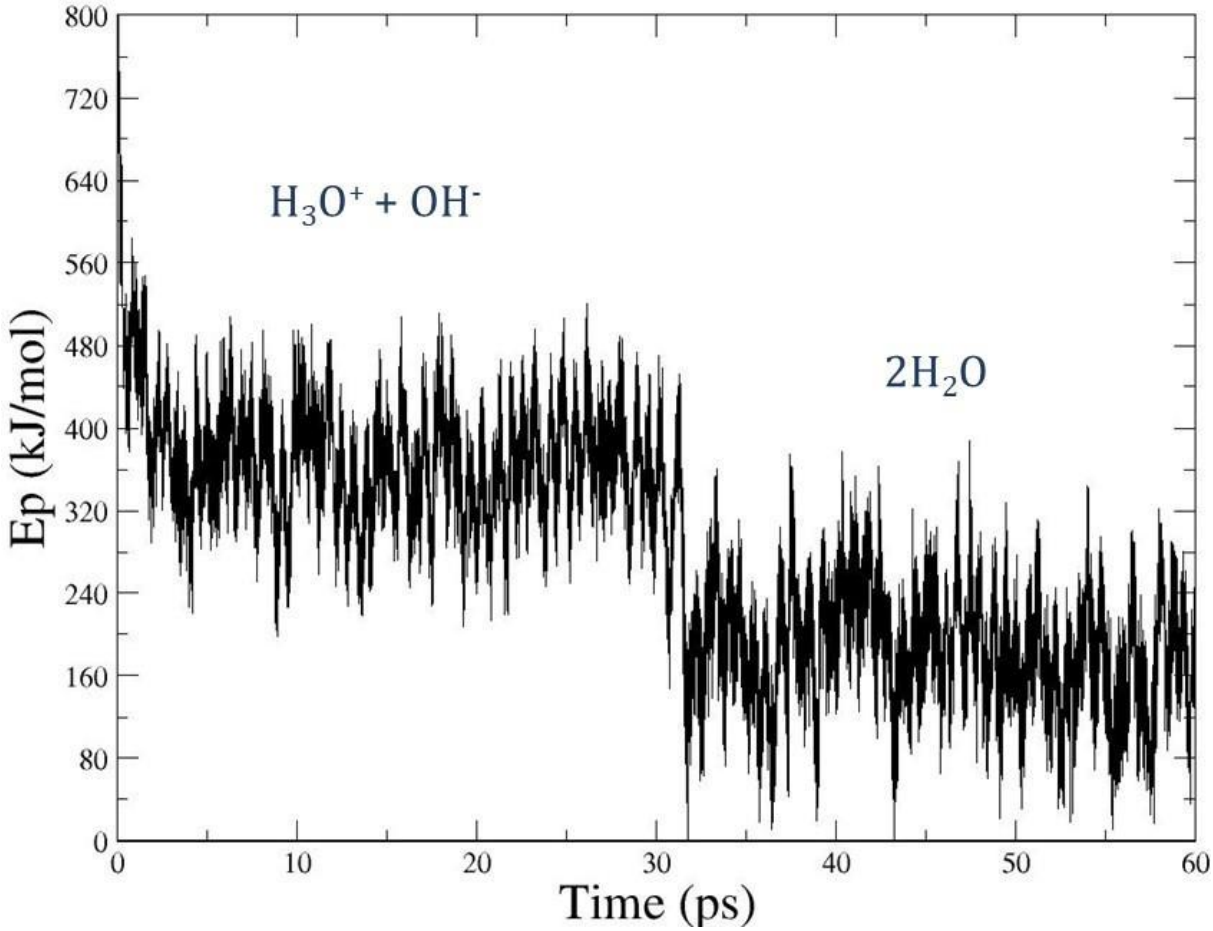


Figure S4- Neutralization reaction at 298 K. Energy values obtained using water-matsci parameter.

3. Proton diffusion coefficient.

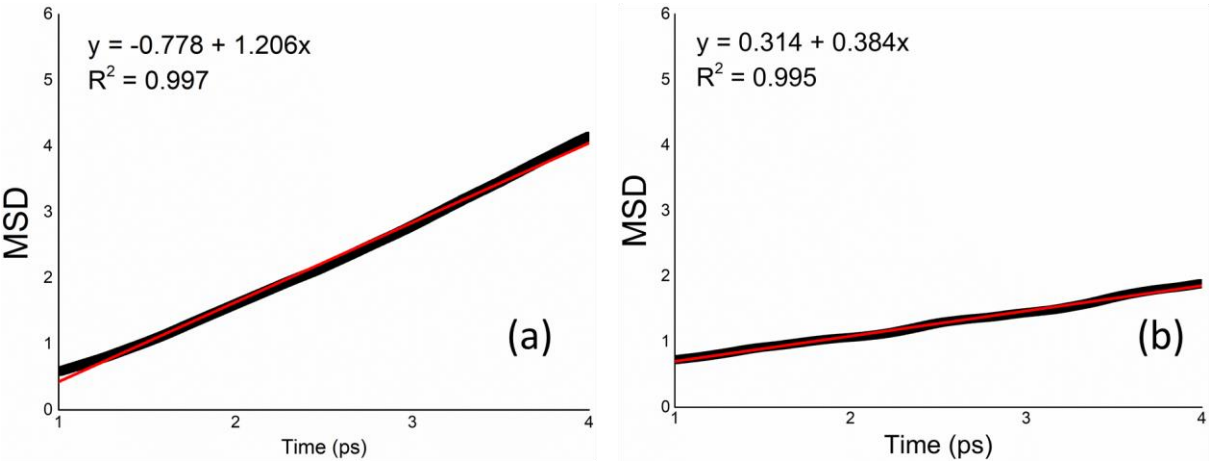


Figure S5. Mean-squared displacements (MSD = $\langle |R(t) - R(t_0)|^2 \rangle$) as functions of time for the proton at 298K for proton (a) and hydronium (b) ions. Values obtained using water-matsci parameter. MSD in Å^2.

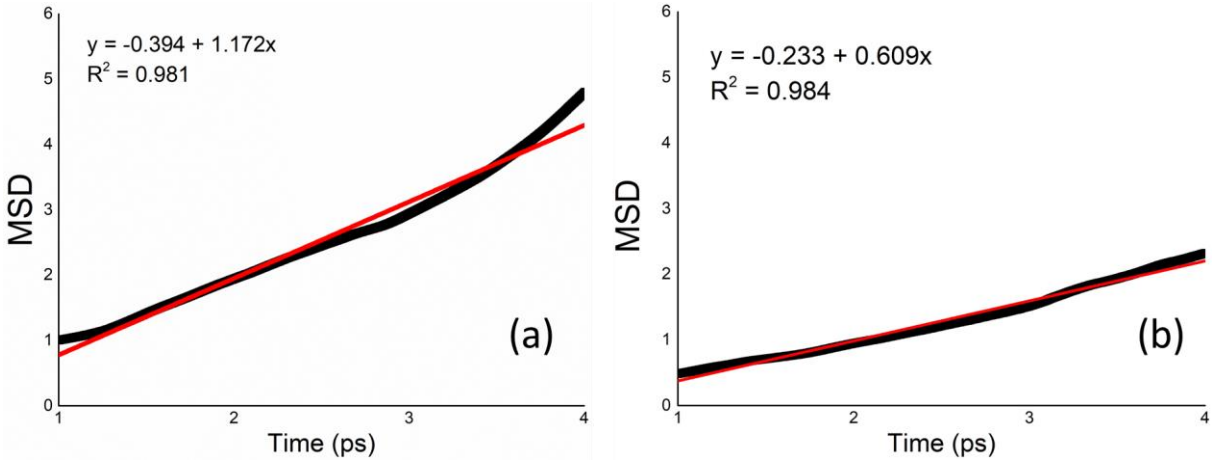


Figure S6. Mean-squared displacements (MSD = $\langle|R(t) - R(t_0)|^2\rangle$) as functions of time for the proton at 298K for proton (a) and hydronium (b) ions. Values obtained using water-matsci-UFF parameter. MSD in Å^2.

4. Lennard-Jones effect in the calculations.

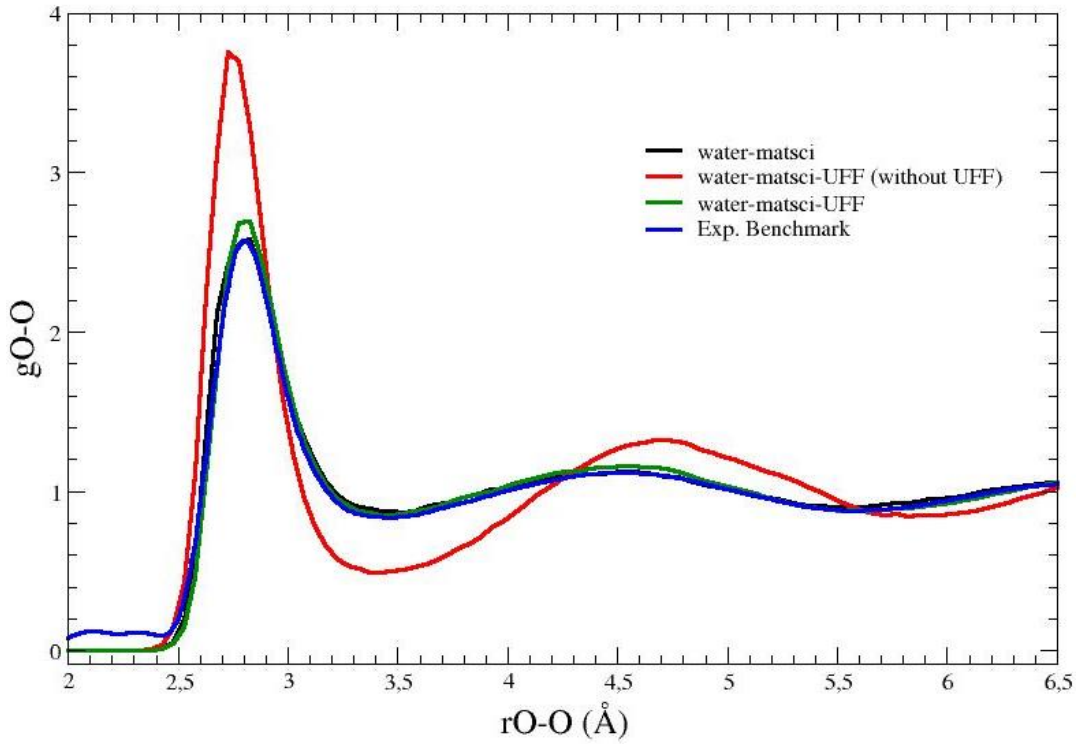


Figure S7. UFF effect in O-O *radial distribution function calculations.*

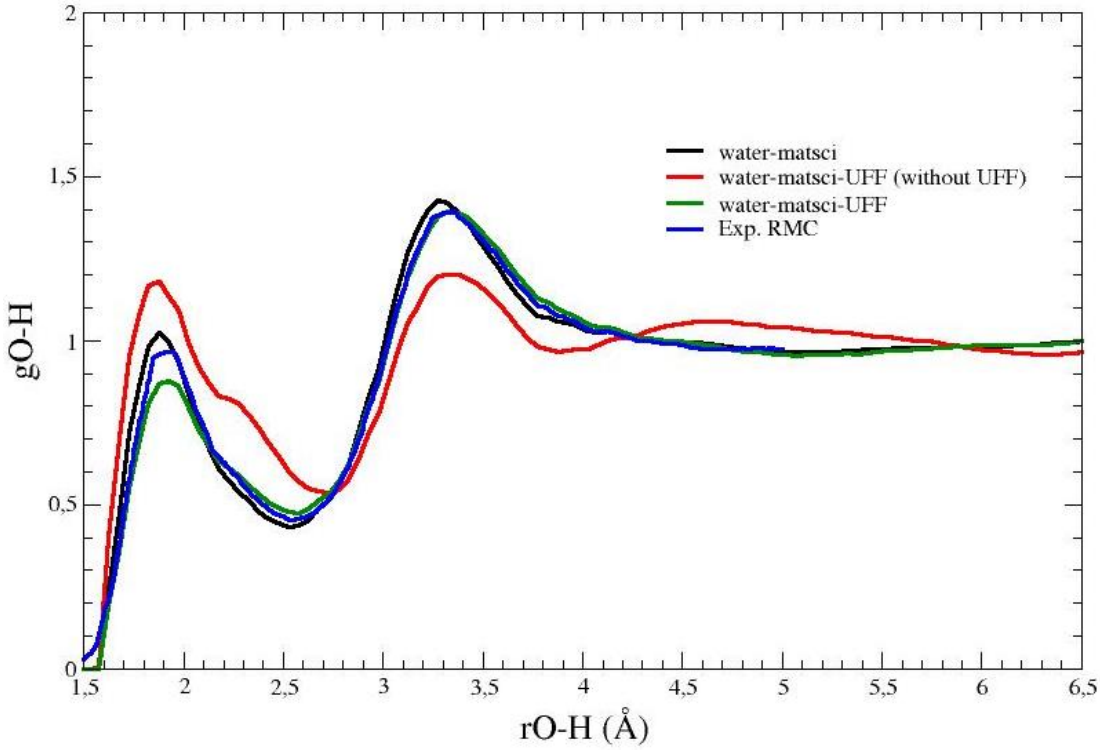


Figure S8. "UFF" effect on O-H *radial distribution function calculations.*

5. Clusters calculations schemes.

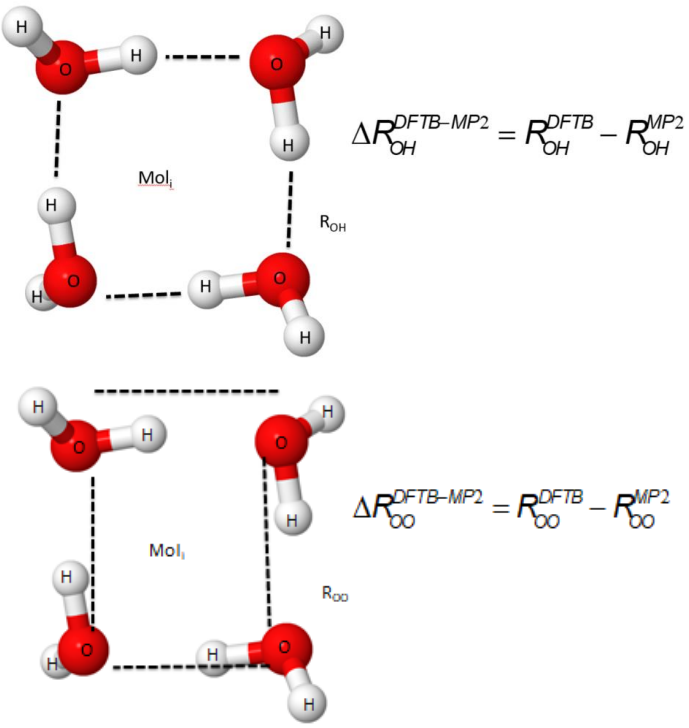


Figure S9. Scheme showing how the O-H and O-O statistics for the clusters were realized.

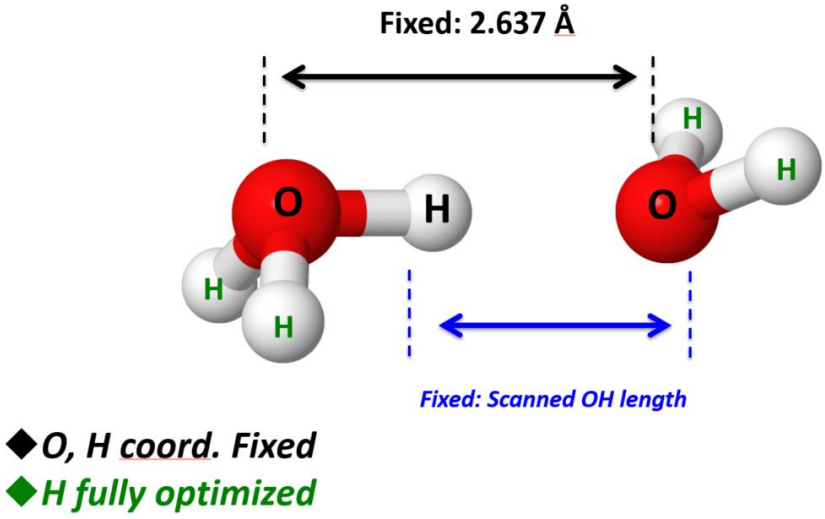


Figure S10. The molecular scheme to obtain the proton transfer potentials. The hydrogen atoms in green were fully optimized and the oxygen atoms in black were fixed while scanning the OH length.

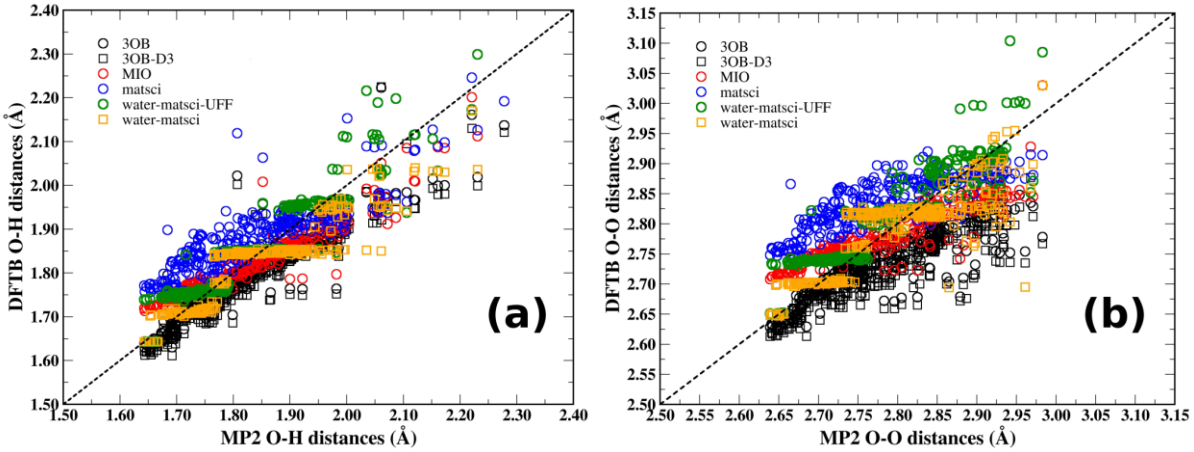


Figure S11. O-H (a) and (O-O) (b) correlation distances (Å) between the CCSD/CBS and different DFTB methods and parameterization for the 38 clusters with 2 to 10 water molecules[17] as well as the hexamers (book, cage, cyclic and prism).

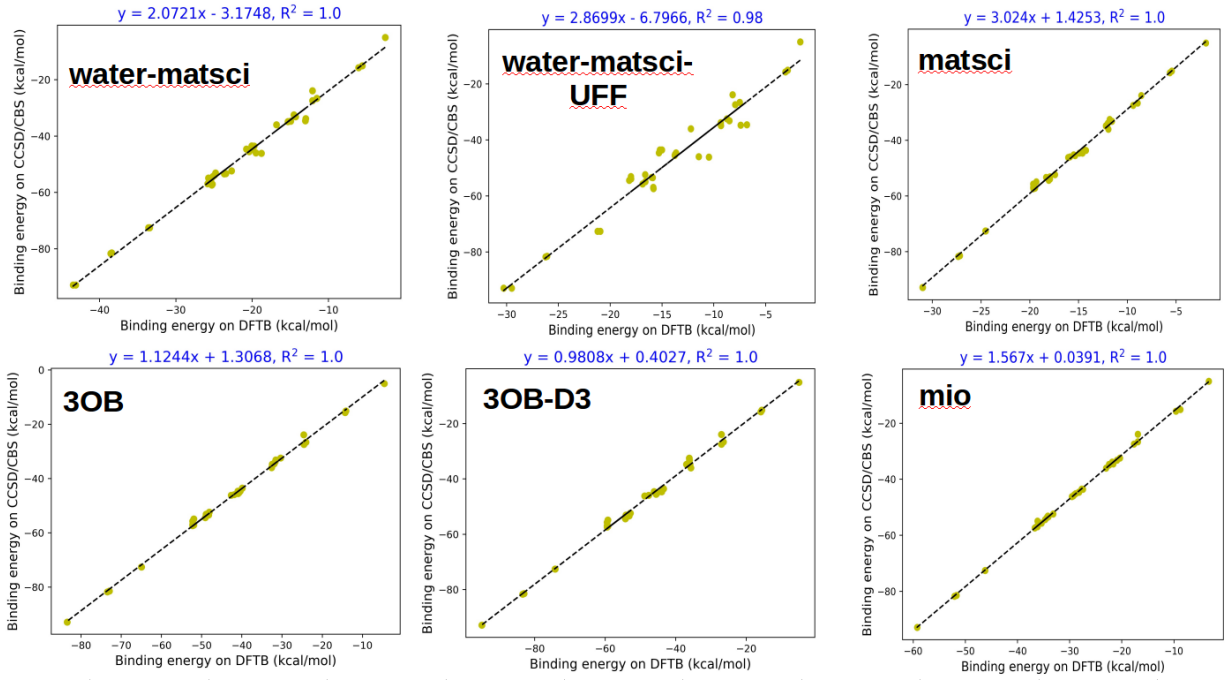
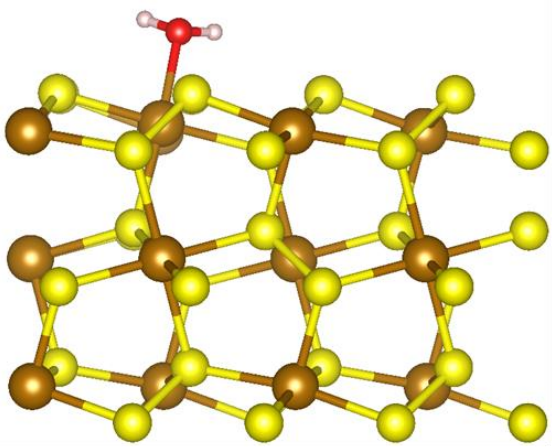


Figure S12. Linear correlation fit for the clusters binding energies for several DFTB methods/ parameterization as a function of the the CCSD/CSB ones.

6. Water adsorption on the pyrite (100) surface.



a)

Figure S13- Water adsorption on pyrite (100) surface. Color code: yellow, sulfur; rust, iron; red, oxygen; and white, hydrogen.

7. References

1. Seifert, G.; Vietze, K.; RLCAO program; Technische Universitaet-Dresden; Not Published, 1993.

2. Guimarães, L.; Enyashin, A. N.; Frenzel, J.; Heine, T.; Duarte, H. A.; Seifert, G. Imogolite nanotubes: stability, electronic, and mechanical properties. *ACS Nano* **2007**, 1, 362-368.

3. Lourenço, M. P. Universidade Federal de Minas Gerais, PhD. Thesis, 2013 (http://www.qui.ufmg.br/~duarteh/teses/Tese-Maicon_P_Lourenco.pdf).

4. Koskinen, P.; Mäkinen, V. Density-functional tight-binding for beginners. *Comput. Mater. Sci.* **2009**, *47*, 237-253.

5. Oliveira, A. F.; Seifert, G.; Heine, T.; Duarte, H. A. Density-Functional Based Tight-Binding: an Approximate DFT Method. *J. Braz. Chem. Soc.* **2009**, *20*, 1193-1205.