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Addition/Correction

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Correction to "Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory"

Mauro Del Ben,* Mandes Schönherr,* Jürg Hutter,* and Joost VandeVondele*

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The radial distribution functions for oxygen−oxygen ($g_{OO}(r)$) and oxygen−hydrogen ($g_{OH}(r)$) presented and discussed were incorrectly normalized using the experimental density. In Figure 1 and Table 1, which replace Figure 2 and Table 1 of the original paper,[1] we instead properly take the instantaneous density as obtained during the *NpT* simulation into account for this analysis. The main effect is a rescaling of the $g(r)$ roughly proportional to the ratio of the experimental and computed average density, while the shape remains basically unchanged. For BLYP, the effect is thus on the order of 20%, and the recomputed $g(r)$ and coordination number (3.9) are now in much better agreement with those reported by Schmidt and

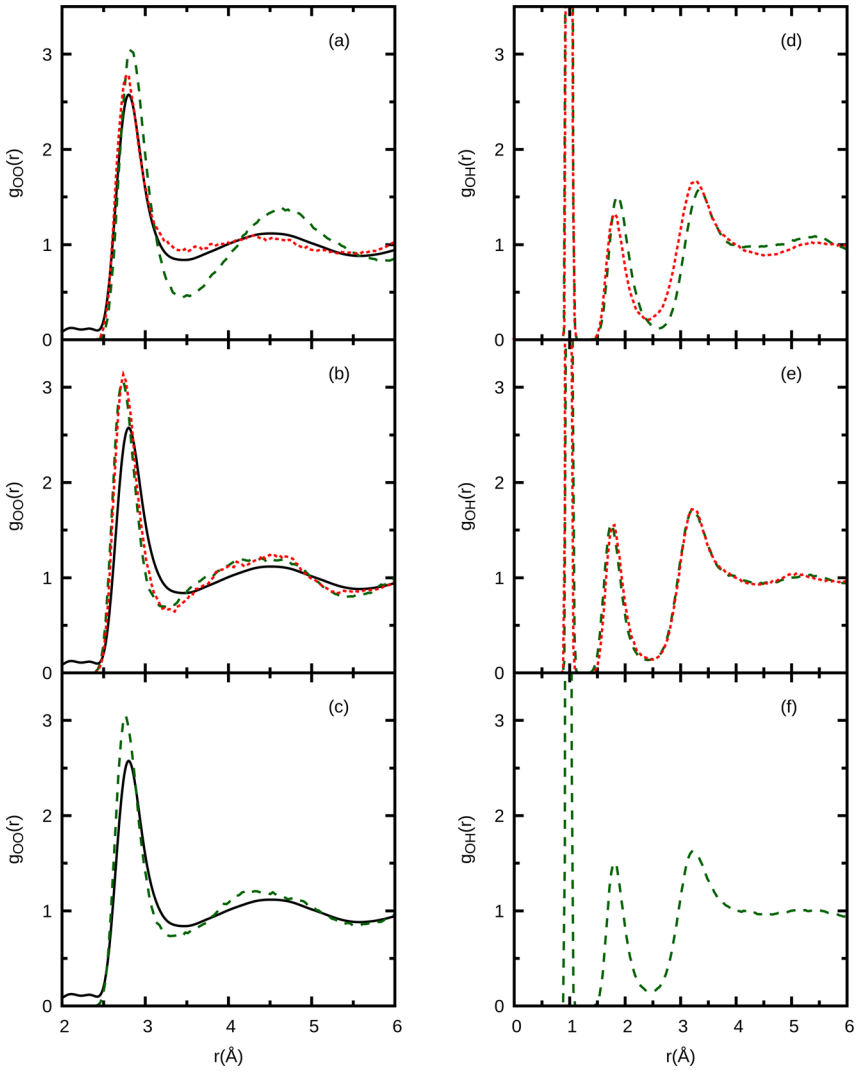

Figure 1. RDFs for oxygen−oxygen (left) and oxygen−hydrogen (right) distances obtained from the *NpT*-MC simulations at the various levels of theory considered (T = 295 K and p = 1 bar). (a,d) BLYP (green dashed) and BLYP-D3 (red dotted); (b,e) PBE-D3 (green dashed) and PBE0-ADMM-D3 (red dotted); (c,f) RI-MP2 (green dashed line). The most recent experimental oxygen−oxygen RDF, obtained from X-ray diffraction and taken from ref 3, is depicted as a solid black line.

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Table 1. Average Density and Structural Data Obtained from the MC *NpT* Simulations at the Various Levels of Theory Considered (T = 295 K and p = 1 bar)[a]

	density [g/mL]		1st max		1st min		2nd max		CN
	ρ	RMSD	r[Å]	$g_{OO}(r)$	r[Å]	$g_{OO}(r)$	r[Å]	$g_{OO}(r)$	n_{OO}
BLYP	0.797	0.018	2.83	3.04	3.46	0.44	4.65	1.37	3.9
BLYP-D3	1.066	0.018	2.78	2.78	3.51	0.92	4.37	1.11	5.9
PBE-D3	1.055	0.015	2.73	3.07	3.25	0.69	4.43	1.21	4.2
PBE0-ADMM-D3	1.023	0.013	2.74	3.13	3.30	0.65	4.52	1.25	4.4
RI-MP2	1.020	0.015	2.76	3.05	3.32	0.72	4.41	1.21	4.5
exp.	1.00		2.80	2.57	3.45	0.84	4.5	1.12	4.3

[a]Experimental values taken from ref 3. CN is the average coordination number calculated from the integral $4\pi\rho_n r^2 g_{OO}(r)$ up to the first minimum, where ρ_n is the average number density of oxygen atoms.

co-workers[2] for *NpT*-based molecular dynamics with the same functional. For those methods that reproduce the experimental density relatively well (PBE0-ADMM-D3, PBE-D3, BLYP-D3) and in particular for RI-MP2, the effect is minimal. This erratum does not affect conclusions reported in the original paper and affects the text only in the second to last paragraph when structural parameters from Table 1 are reported explicitly.

REFERENCES

(1) Del Ben, M.; Schönherr, M.; Hutter, J.; VandeVondele, J. Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory. *J. Phys. Chem. Lett.* **2013**, *4*, 3753−3759.

(2) Schmidt, J.; VandeVondele, J.; Kuo, I.-F. W.; Sebastiani, D.; Siepmann, J. I.; Hutter, J.; Mundy, C. J. Isobaric−Isothermal Molecular Dynamics Simulations Utilizing Density Functional Theory: An Assessment of the Structure and Density of Water at Near-Ambient Conditions. *J. Phys. Chem. B* **2009**, *113*, 11959−11964.

(3) Skinner, L. B.; Huang, C.; Schlesinger, D.; Pettersson, L. G. M.; Nilsson, A.; Benmore, C. J. Benchmark Oxygen−Oxygen Pair-Distribution Function of Ambient Water from X-ray Diffraction Measurements with a Wide Q-Range. *J. Chem. Phys.* **2013**, *138*, 074506.

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