Supplementary Materials

Development of Polarizable Models for Molecular Mechanical Calculations III: Polarizable Water Models Conforming to Thole Polarization Screening Schemes

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Table S1. Second virial coefficients for the POL3-LT water model calculated using 3-, 5- and 7-point Gauss quadratures.

TEMP	3p-Gauss	5p-Gauss	7p-Gauss
273.15	-2303.1	-2309.5	-2309.5
293.15	-1493.2	-1497.0	-1497.0
295.15	-1435.7	-1439.3	-1439.3
298.15	-1355.2	-1358.5	-1358.6
323.15	-881.4	-883.3	-883.3
373.15	-455.3	-456.0	-456.0
423.15	-277.8	-278.1	-278.1
448.15	-225.8	-226.1	-226.1
473.15	-187.1	-187.3	-187.3
523.15	-134.2	-134.3	-134.3
573.15	-100.2	-100.3	-100.3
673.15	-60.2	-60.2	-60.2
773.15	-38.0	-38.0	-38.0
873.15	-24.2	-24.2	-24.2
973.15	-14.9	-14.9	-14.9
1000	-12.9	-12.9	-12.9
1100	-6.9	-6.9	-6.9
1200	-2.4	-2.4	-2.4
1300	1.0	1.0	1.0
1400	3.7	3.7	3.7

Table S2. Comparison between simulations with different number of water molecules and cutoff.

Model	ρ	ΔH_{vap}	D	ε_0
POL3(small)	1.002(0.000)	10.46(0.00)	2.4(0.1)	125(2)
POL3 (large)	1.001(0.000)	10.45(0.00)	2.5(0.1)	126(3)

Densities (ρ , g/cm^3), enthalpies of vaporization (ΔH_{vap} , kcal/mol), diffusion constants (D , 10^{-9} m^2/s), dielectric constants (ε_0) for the POL3 water model at 298 K and 1 atm. Small: No_{water} = 499, cutoff = 9 Å; Large: No_{water} = 2031, cutoff = 15 Å. The numbers in parentheses are the standard deviations.

Table S3. Self-diffusion coefficients of water models at 200K, 230K, and 298K.

Model	200K	230K	298K
POL3	0.01(0.00)	0.17(0.01)	2.4(0.1)
POL3-LT	0.01(0.00)	0.16(0.00)	2.5(0.1)
POL3-ET	0.01(0.00)	0.17(0.01)	2.6(0.1)
DA/DA-LT	0.01(0.00)	0.08(0.00)	1.8(0.0)
DA-ET	0.01(0.00)	0.08(0.00)	1.9(0.1)
NDA/NDA-LT	0.01(0.00)	0.23(0.01)	2.7(0.0)
NDA-ET	0.01(0.00)	0.24(0.01)	2.7(0.0)
DC/DC-LT	0.01(0.00)	0.09(0.01)	2.3(0.1)
DC-ET	0.01(0.00)	0.09(0.00)	2.4(0.1)

Table S4. Second virial coefficient for polarizable water models studied in this work.

TEMP	EXP.	POL3	POL3-LT	POL3-ET	DC/DC-LT	DA/DA-LT/ET	NDA/NDA-LT/ET	TIP4P	CC-pol
273.15	-1916.9	-2310.3	-2309.5	-2310.2	-1187.1	-1923.9	-1790.9	-7647.5	-2360.8
293.15	-1307.8	-1497.5	-1497	-1497.5	-834.4	-1277.6	-1200.5	-4428.3	-1572.0
295.15	-1262.9	-1439.8	-1439.3	-1439.7	-807.9	-1230.9	-1157.6	-4213.8	-1514.9
298.15	-1199.7	-1359	-1358.5	-1359	-770.5	-1165.4	-1097.3	-3917.5	-1434.6
323.15	-816.7	-883.6	-883.3	-883.5	-539.4	-773.9	-735.1	-2275	-954.4
373.15	-451.6	-456.2	-456	-456.2	-307.4	-410.6	-394.7	-995.1	-507.8
423.15	-289.9	-278.2	-278.1	-278.2	-198.8	-254.5	-246.4	-544.6	-316.2
448.15	-240.6	-226.1	-226.1	-226.1	-164.9	-208.0	-201.9	-425.6	-259.4
473.15	-203.2	-187.4	-187.3	-187.4	-138.8	-173.2	-168.4	-341.6	-216.9
523.15	-150.5	-134.3	-134.3	-134.3	-101.7	-125	-121.9	-233.7	-158.3
573.15	-115.7	-100.3	-100.3	-100.3	-76.9	-93.8	-91.6	-169.4	-120.5
673.15	-73.6	-60.2	-60.2	-60.2	-46.4	-56.7	-55.4	-99.2	-75.8
773.15	-49.7	-38.0	-38.0	-38.0	-28.8	-35.9	-35.0	-63.0	-50.8
873.15	-34.6	-24.2	-24.2	-24.2	-17.6	-22.9	-22.2	-41.6	-35.2
973.15	-24.4	-14.9	-14.9	-14.9	-9.9	-14.0	-13.5	-27.8	-24.6
1000	-22.2	-12.9	-12.9	-12.9	-8.2	-12.2	-11.6	-24.9	-22.4
1100	-15.5	-6.9	-6.9	-6.9	-3.1	-6.4	-5.9	-16.2	-15.4
1200	-10.4	-2.4	-2.4	-2.4	0.8	-2.0	-1.6	-9.9	-10.2
1300	-6.5	1.0	1.0	1.0	3.7	1.3	1.7	-5.1	-6.2
1400	-3.4	3.7	3.7	3.7	6.1	3.9	4.3	-1.4	-3.0
χ^2		216.4	215.6	216.3	1117.8	87.9	143.4	41434.9	288.2

Comparison with experimental data, measured by χ^2 value defined in the main text.

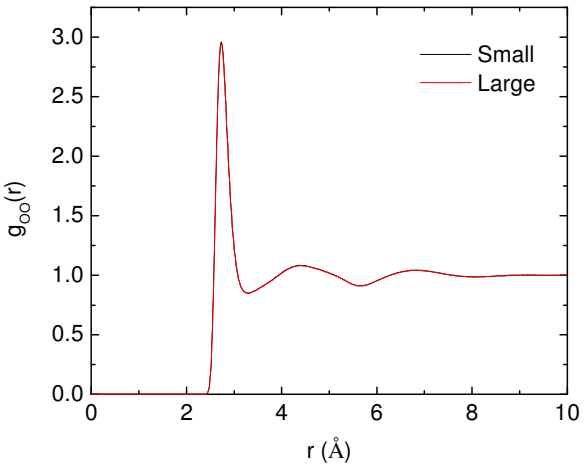

Figure S1. Radial distribution functions of the POL3 water model generated by different simulations with different number of water molecules and cutoff. Small: No_{water} = 499, cutoff = 9 Å; Large: No_{water} = 2031, cutoff = 15 Å.

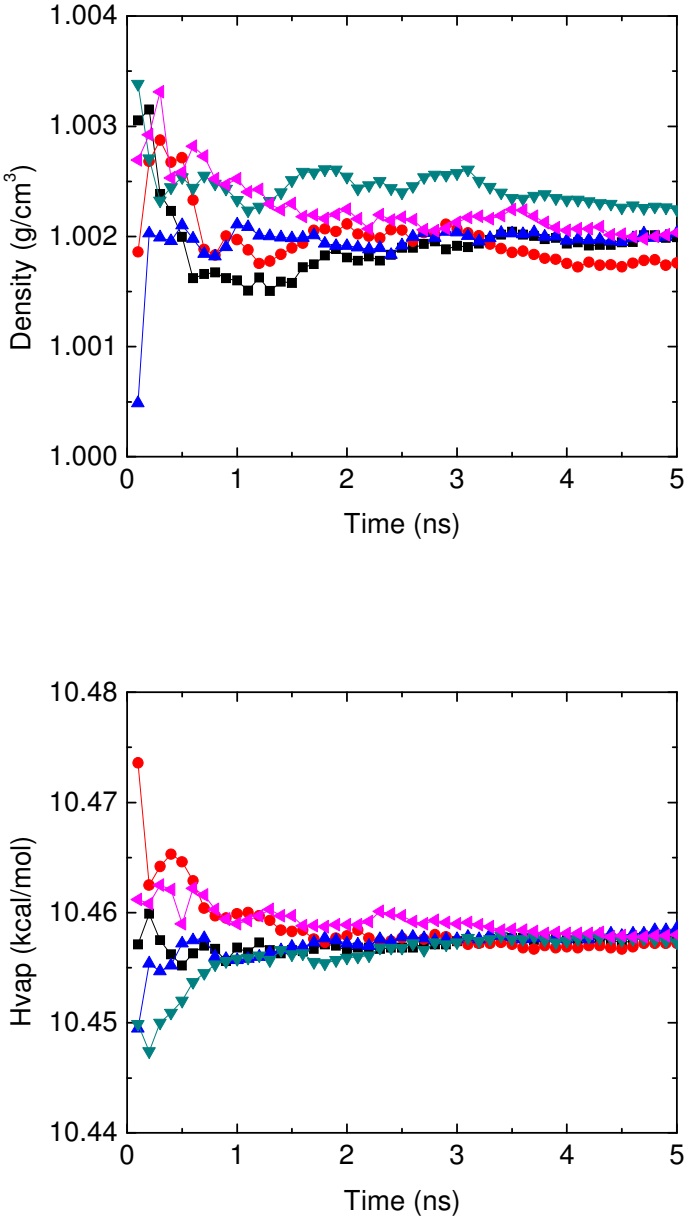

Figure S2. Cumulative averages of Density and Hvap of the POL3 model (No_{water} = 499, cutoff = 9 Å). Here different colors represent different trajectories. The final values are averaged over all five trajectories.

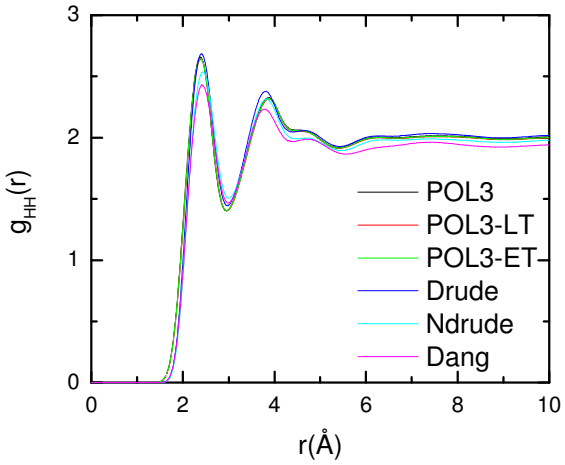

Figure S3. Comparison of simulated radial distribution functions $g_{HH}(r)$ for tested polarizable water models.

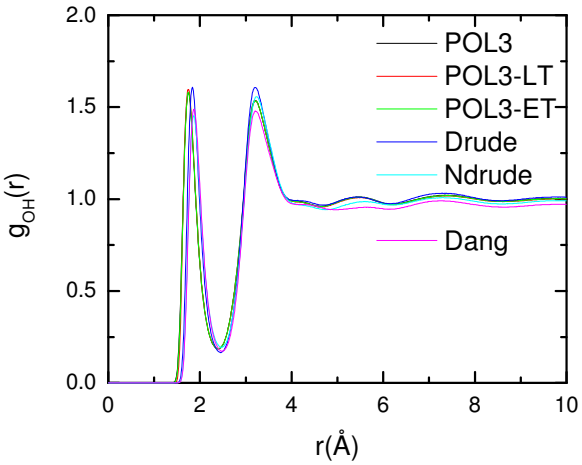

Figure S4. Comparison of simulated radial distribution functions $g_{OH}(r)$ for tested polarizable water models.

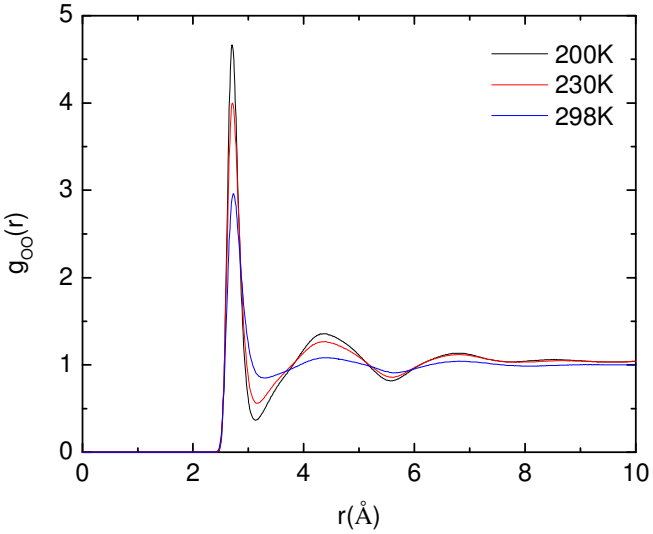

Figure S5. Comparison of simulated radial distribution functions $g_{OO}(r)$ at three simulated temperatures for the POL3 water model.

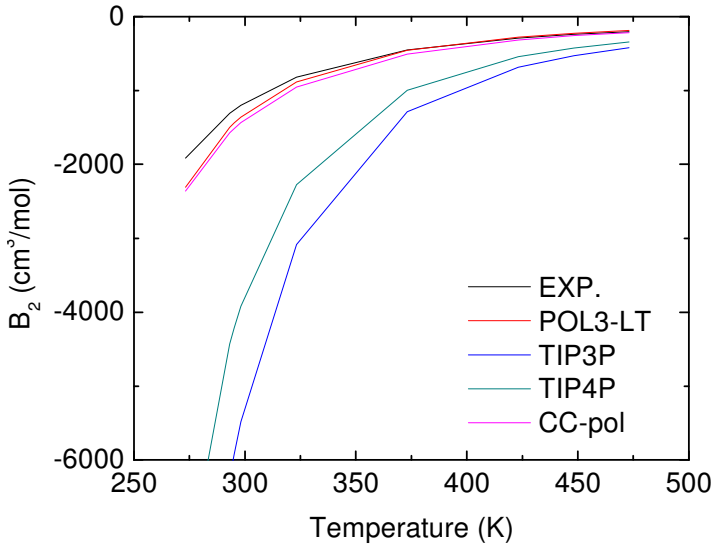

Figure S6. The second virial coefficients as a function of temperature. Comparison of POL3-LT with two popular TIP3P and TIP4P additive models and quantum mechanical CC-pol model.