

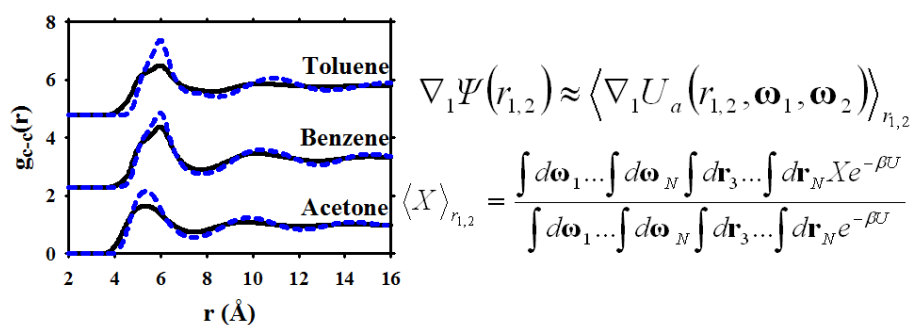
Role of short-range directional interactions in coarse-graining of protic/aprotic liquids

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To estimate the accuracy of the proposed Monte Carlo (MC) algorithm as well as computational methodology we report thermodynamic and structural properties of liquid water computed from several rigid models of water. Note that from studied liquids, water is the most difficult to simulate because of the short-range directional H-bonds. That is why; we use water for reproduction of the experimental results.

Using MC method implemented in (N,P,T) ensemble, we computed the heat capacity, isothermal compressibility, and the heat of vaporization from the fluctuation formulas¹⁻³,

$$C_p = (\partial \langle H \rangle / \partial T)_{N,p} = (1 / Nk_b T^2) (\langle H^2 \rangle - \langle H \rangle^2) + 3R \quad (1S)$$

$$\kappa = -1/V (\partial \langle V \rangle / \partial p)_{N,T} = (\langle V^2 \rangle - \langle V \rangle^2) / k_b T \langle V \rangle \quad (2S)$$

$$H = E(liq.) + pV = \sum_{a<b} E_{ab} + pV \quad (3S)$$

$$\Delta H_{vap} = E(gas) - E(liq.) + p(V(gas) - V(liq.)) \approx -\langle E(liq.) \rangle / N + RT \quad (4S)$$

Property	TIP4P	SPC/E	TIP5P	SPC	TIP4P-Ew
$d (g\ cm^{-3})$	0.999 ± 0.003	1.005 ± 0.005	0.990 ± 0.004	0.985 ± 0.005	1.004 ± 0.003
$\Delta H_{vap} (kcal / mol)$	10.64 ± 0.01	11.97 ± 0.03	10.48 ± 0.02	10.74 ± 0.02	11.88 ± 0.02
$C_p (cal / mol\ K)$	20.49 ± 1.5	20.23 ± 1.7	25.49 ± 3.3	20.36 ± 2.1	19.34 ± 1.8
$10^6 \kappa (1 / atm)$	44 ± 7	35 ± 10	47 ± 8	49 ± 6	31 ± 11
$E_{pot} (kcal / mol)$	-10.05 ± 0.01	-11.38 ± 0.03	-9.89 ± 0.02	-10.15 ± 0.02	-11.29 ± 0.03

For comparison the experimental values (see Reference 3) ($T = 298\ K$, $p = 1\ atm$) are, $d = 0.997\ g\ cm^{-3}$, $\Delta H_{vap} = 10.51\ kcal\ mol^{-1}$, $C_p = 18.0\ cal\ mol^{-1}\ K^{-1}$, $10^6 \kappa = 45.8\ atm^{-1}$.

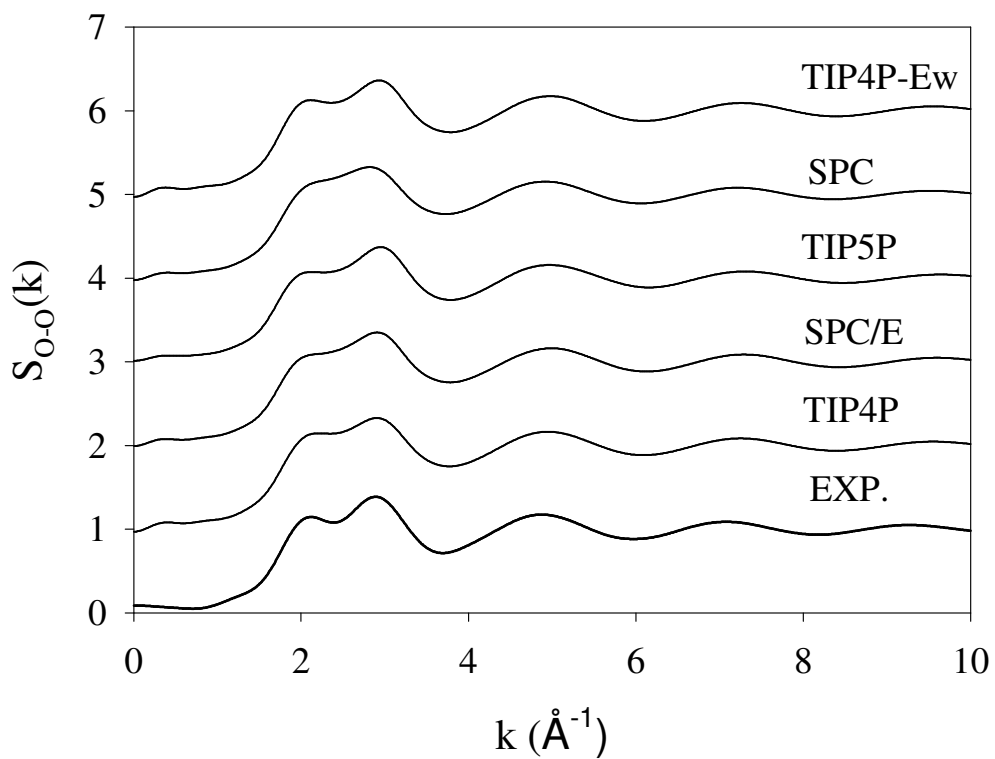


figure 1S. Computed and experimental^{3,4} oxygen-oxygen structure factors for liquid water at 298 K and 1 atm.

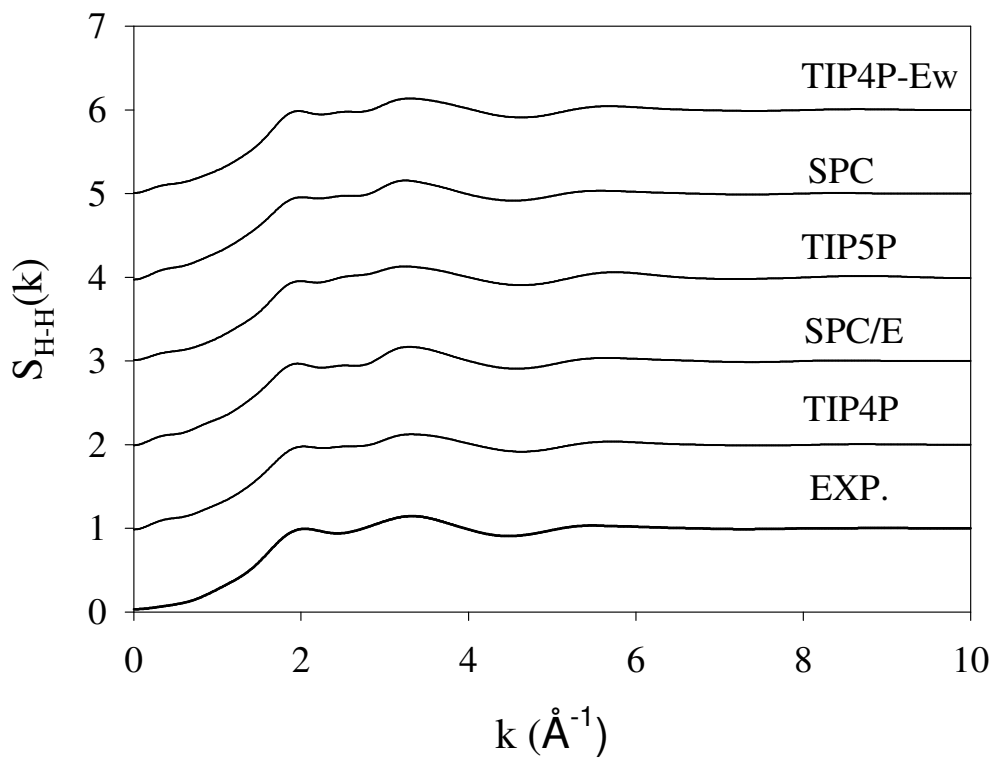


figure 2S. Computed and experimental^{3,4} hydrogen-hydrogen structure factors for liquid water at 298 K and 1 atm.

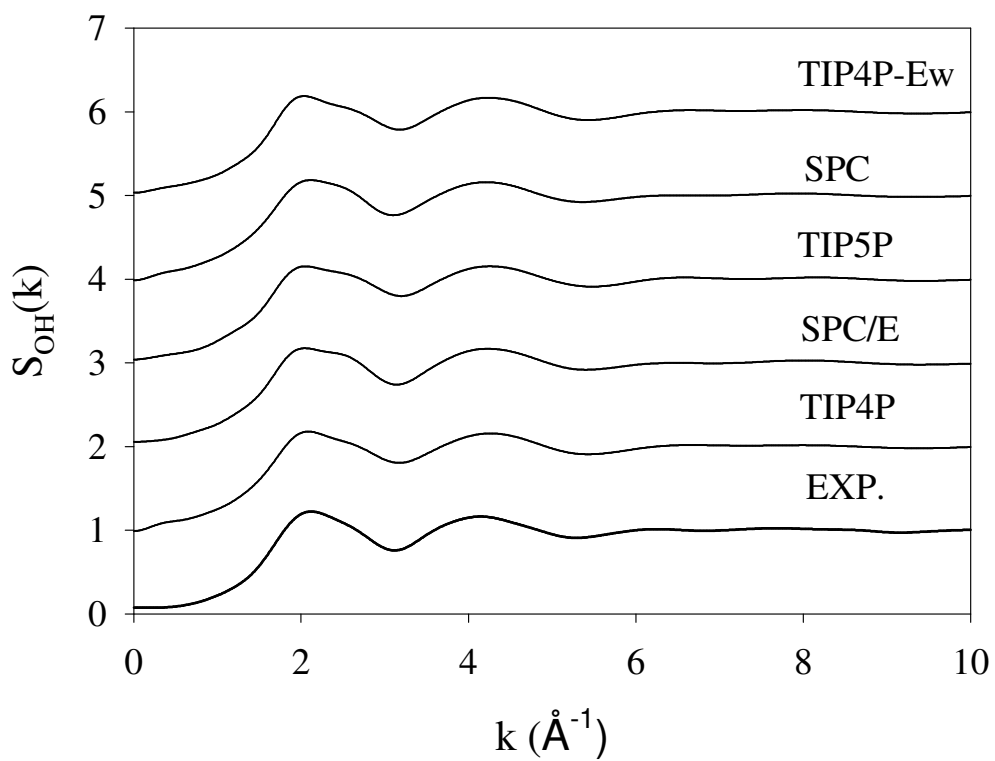


figure 3S. Computed and experimental^{3,4} oxygen-hydrogen structure factors for liquid water at 298 K and 1 atm.

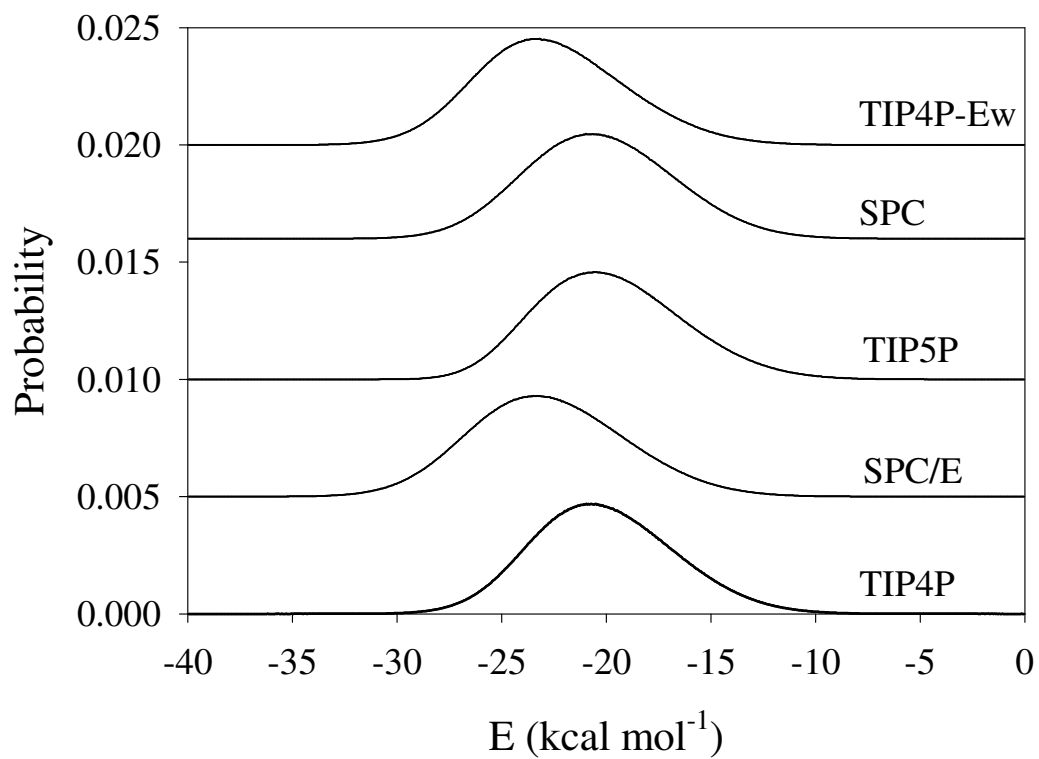


figure 4S. Computed total bonding energy profiles for liquid water monomer at 298 K and 1 atm.

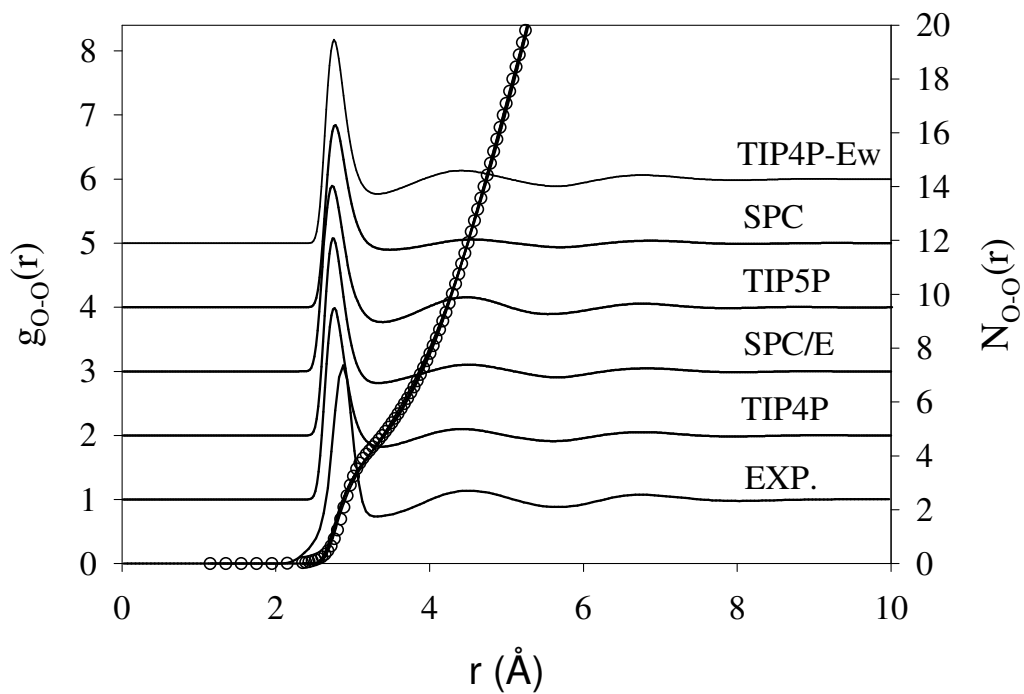


figure 5S. Computed and experimental^{3,4} oxygen-oxygen radial distribution functions and average number of oxygen atoms for liquid water at 298 K and 1 atm.

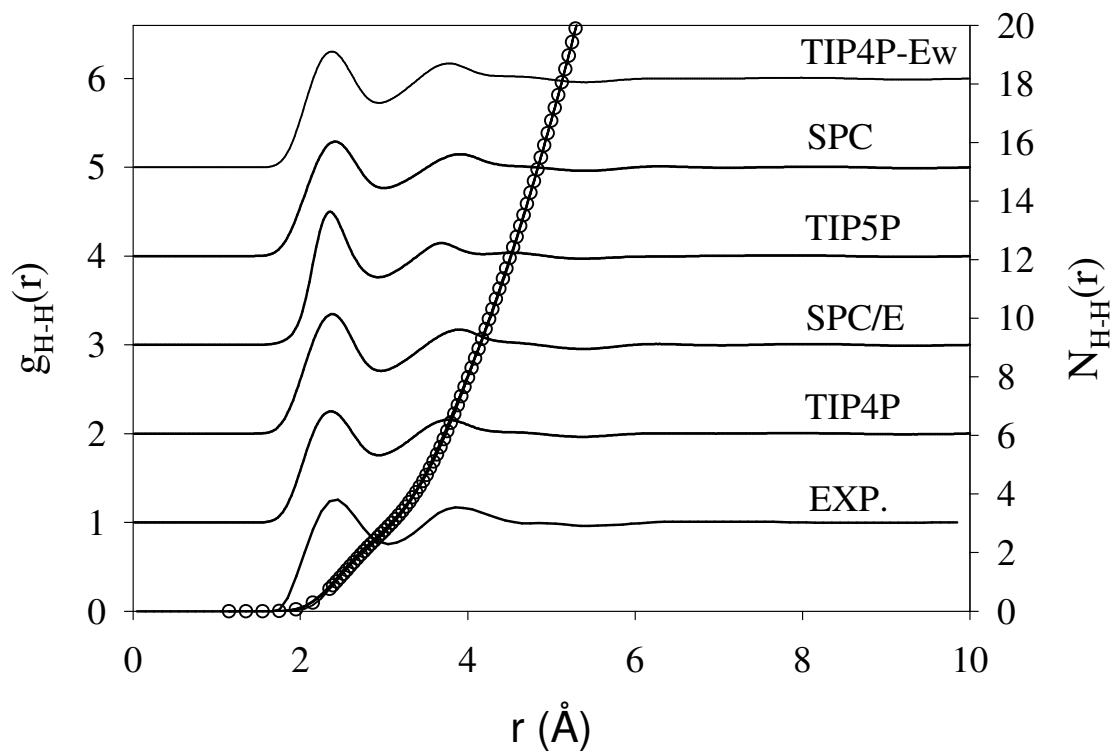


figure 6S. Computed and experimental^{3,4} hydrogen-hydrogen radial distribution functions and average number of hydrogen atoms for liquid water at 298 K and 1 atm.

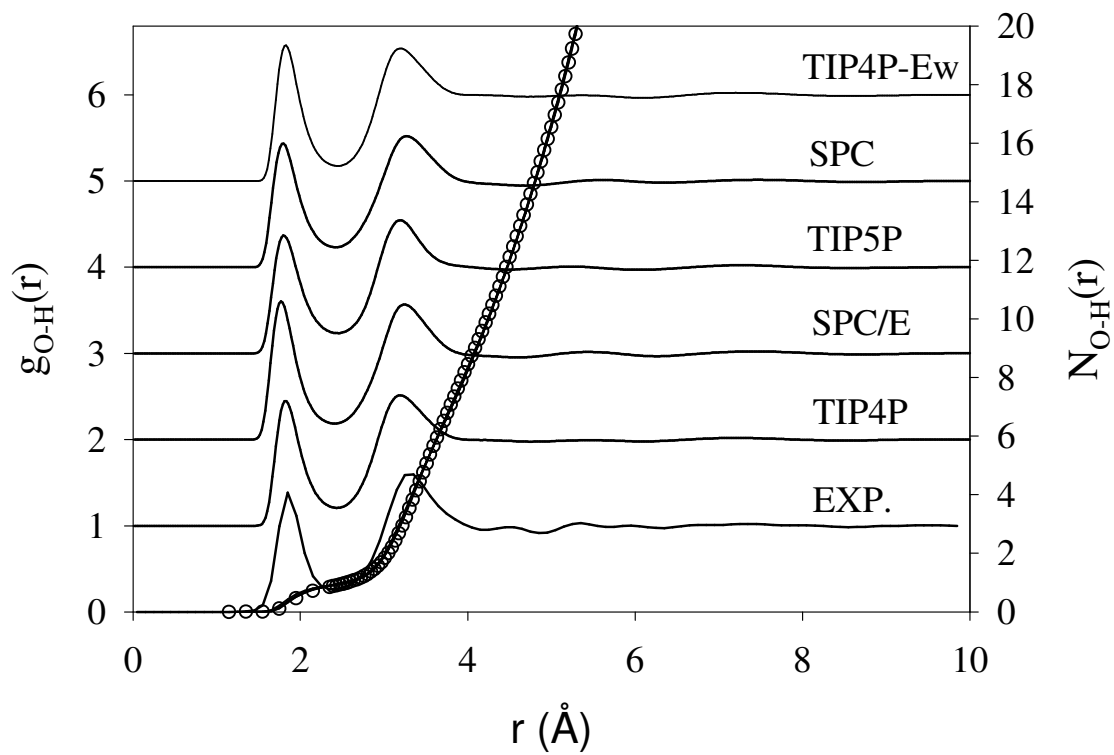


figure 7S. Computed and experimental^{3,4} oxygen-hydrogen radial distribution functions and average number of hydrogen and oxygen atoms for liquid water at 298 K and 1 atm.

References

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- (4) Soper, A. K.; Phillips, M. G. *Chem. Phys.* **1985**, *107*, 471985.