Adaptive resolution simulation of liquid water

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Corrigendum

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Matej Praprotnik, Silvina Matysiak, Luigi Delle Site, Kurt Kremer and Cecilia Clementi
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In our two papers [1, 2], we used a rigid all-atom TIP3P water model with a H-O-H angle of 112.20° instead of, as erroneously stated, the standard rigid TIP3P model [3] with a 104.52° H-O-H angle. All the other parameters are the same as in the standard rigid TIP3P water model. The statistical properties of similarly modified water models have been studied by other authors, cf references [4–6]. Since in the adaptive resolution simulations reported in references [1, 2] the modified TIP3P all-atom water model was studied in combination with the appropriate coarse-grained model, all conclusions of the paper concerning the adaptive resolution simulation remain unaltered.

References

[1] Praprotnik M, Matysiak S, Delle Site L, Kremer K, and Clementi C 2007 *J. Phys.: Condens. Matter* **19** 292201
[2] Matysiak S, Clementi C, Praprotnik M, Kremer K and Delle Site L 2008 *J. Chem. Phys.* **128** 024503
[3] Jorgensen W L, Chandrasekhar J, Madura J D, Impey R W and Klein M L 1983 *J. Chem. Phys.* **79** 926
[4] Höchtl P, Boresch S, Bitomsky W and Steinhauser O 1998 *J. Chem. Phys.* **109** 4927
[5] Wu Y, Tepper H L and Voth G A 2006 *J. Chem. Phys.* **124** 024503
[6] Chatterjee S, Debenedetti P G, Stillinger F and Lynden-Bell R M 2008 *J. Chem. Phys.* **128** 124511

