ADDITIONS AND CORRECTIONS

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Jürgen Köfinger and Christoph Dellago*: Biasing the Center of Charge in Molecular Dynamics Simulations with Empirical Valence Bond Models: Free Energetics of an Excess Proton in a Water Droplet

Due to a typesetting error, eq 18 on p 2351 of our recent paper[1] was incorrectly published as

$$\frac{\partial c_{0i}}{\partial x^{\alpha}} = \sum_{j\neq 0} \sum_{l,m} \frac{D^{\alpha}_{lm} c_{jl} c_{0m}}{E_0 - E_j} \tag{1}$$

The correct equation is

$$\frac{\partial c_{0i}}{\partial x^{\alpha}} = \sum_{j\neq 0} \sum_{l,m} \frac{D^{\alpha}_{lm} c_{jl} c_{0m}}{E_0 - E_j} c_{ji} \tag{2}$$

The correct equation was used in all calculations. Also, all equations derived from eq 18 of our original article are correct.

Equation 2 is central to the calculation of forces in biased molecular dynamics simulations of proton transfer based on the multistate valence bond model of Voth and collaborators.[2] We would like to point out that this result was published earlier in ref 3 (see eqs 6 and 7) by H. L. Tepper and G. A. Voth who attributed it to A. M. Smondryev and G. A. Voth citing unpublished work. We were not aware of this article at the time of publication of our paper.[1]

References and Notes

(1) Köfinger, J.; Dellago, C. *J. Phys. Chem. B* **2008**, *112*, 2349–2356.
(2) Schmitt, U. W.; Voth, G. A. *J. Phys. Chem. B* **1998**, *102*, 5547.
(3) Tepper, H. L.; Voth, G. A. *Biophys. J.* **2005**, *88*, 3095–3108.

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