

**Reply to “Comment on ‘Molecular Dynamics Simulation of the Liquid/Vapor Interface of Aqueous Ethanol Solutions as a Function of Concentration’”**

Ramona S. Taylor

*Spectral Sciences, Inc., Burlington, Massachusetts 01803*

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Overall, I think that the comment of Wang et al.<sup>1</sup> offers an interesting alternative for defining concentration in molecular dynamics simulations of liquid solutions. Traditionally, in both simulation and experiment, concentration has been defined as the number of moles of constituent A versus the number of moles of constituent B in a given volume. Wang et al. suggest that that this definition may not be appropriate in molecular dynamics simulations of surface active species where a liquid/vapor interface is present due to the finite size of the simulation

box and the propensity for one of the two components (either A or B) to want to reside at the interface. Instead, they suggest that one should define the solution concentration as the concentration measured in the bulk-like regions of the simulation cell. This is quite an interesting idea. In fact, when it is applied to simulation data for aqueous ethanol solutions of Stewart et al.<sup>2</sup>, it leads to much better agreement between the experimental and simulation surface tension data. In addition, it also leads to better agreement between the experimental and simulation surface excess data (see ref 8 of Stewart et al.<sup>2</sup>). Finally, it would be interesting to test whether the authors' new definition of concentration is capable of explaining the differences between other experimental and simulation results.

**References and Notes**

- (1) Wang, J.; Wang, T. *J. Phys. Chem. B* **2005**, *109*, 22699.
- (2) Stewart, E.; Shields, R. L.; Taylor, R. S. *J. Phys. Chem. B* **2003**, *107*, 2333.