Correction to "Ab Initio Molecular Dynamics Approach to Quantitative Description of Ion Pairing in Water"

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We have found a trivial numerical error, a redundant multiplicative factor of 2, in our script for evaluation of the mean force and the potential of the mean force from the ab initio molecular dynamics, presented in Figure 1 in our Letter. A corrected Figure 1 is presented below. No results from
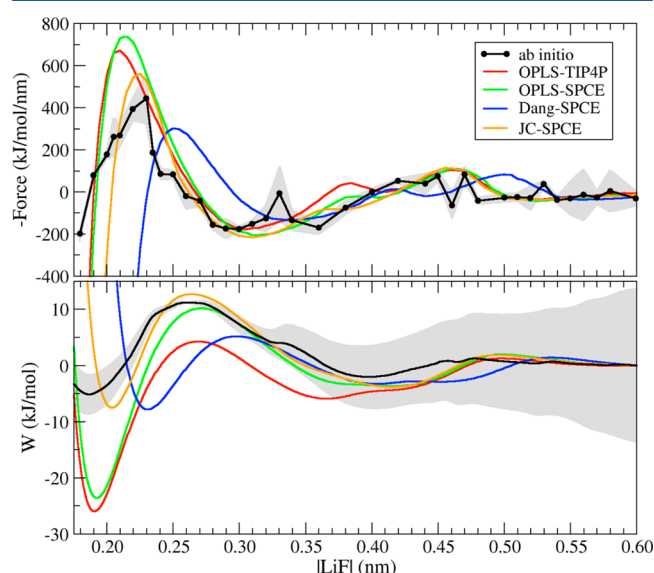

Figure 1. Negative of the mean force (upper part) and integral thereof with entropic correction, that is, the PMF (lower part) along the Li−F coordinate. Ab initio mean forces (black circles) were calculated for 38 points corresponding to 50 ps trajectories after 5 ps of equilibration. The gray area in the upper part indicates the statistical error in force evaluation estimated by the block average analysis method, which being integrated gives an upper bound to the error of the PMF (gray area in the lower part). Comparison is made to 10 ns trajectories per point for the same system simulated using four different empirical force fields (colored lines). All free-energy profiles are normalized to zero at the largest investigated ion−ion separation.

classical force field simulations are affected. Also, the positions of stationary points on the ab initio free-energy curve remain the same. However, as a result of the correction to the ab initio potential of mean force, the transition state on the free-energy curve is now only 16 kJ/mol above the contact ion pair, and our previous conclusion that the classical force fields strongly underestimate this barrier is no longer valid.

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