

ADDITIONS AND CORRECTIONS

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T. Werder, J. H. Walther, R. L. Jaffe, T. Halicioglu, and P. Koumoutsakos*: On the Water–Carbon Interaction for Use in Molecular Dynamics Simulations of Graphite and Carbon Nanotubes

Page 1349. A conversion error has been detected in the analysis of the line tension (Figure 4); the units of the abscissa axis should be \AA^{-1} . The subsequent analysis of the line tension on page 1349 is therefore in error by a factor of 10. Thus, the magnitude of the line tension can be estimated from the slopes of the fits in Figure 1, compare eq 3, which are -0.94 (case 14), -3.33 (case 1), and -3.72 \AA (case 10), respectively. For a surface tension of water of $\gamma_{LV} = 72 \text{ mN/m}$, the line tension τ is found to be 0.7×10^{-11} (case 14), 2.4×10^{-11} (case 1), and $2.7 \times 10^{-11} \text{ J/m}$ (case 10). This error has no implication for the remaining analysis and conclusions presented in the paper. A corrected version of Figure 4 is given below.

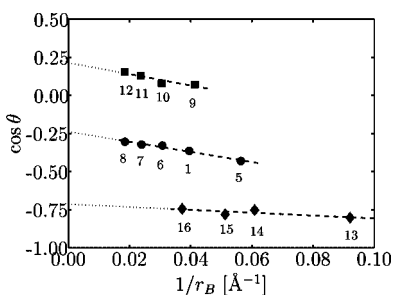


Figure 4. Cosine of the contact angle θ as a function of the droplet base curvature $1/r_B$. The three series are computed using Lennard-Jones parameters of $\epsilon_{CO} = 0.3135$ (circles), 0.4389 (squares), and $0.1881 \text{ kJ mol}^{-1}$ (diamonds) for droplets with an increasing number of water molecules: 1000 (cases 5, 13, and 9), 2000 (cases 1, 14, and 10), 4000 (cases 6, 15, and 11), 8379 (case 7, 16, and 12), and 17576 (case 8).

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