Macromolecules

ADDITION/CORRECTION

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Polyelectrolyte Brushes: MD Simulation and SCF Theory
[*Macromolecules* **2010**, *43*, 7845–7851]. Su-zhen He, Holger Merlitz,* Long Chen, Jens-Uwe Sommer, and Chen-Xu Wu*

Page 7846. In the original submission we describe a method to determine the Kuhn length of our coarse-grained polymer model. Though this approach was also used in ref 25, it did not deliver reliable results. Within the SCF formalism [ref 17], b is defined for the corresponding ideal chain model, which would be $b = 1$ in our case, but in good solvent this value is inaccurate due to local excluded volume interactions. We found that a most consistent result is achieved by fitting the effective b to the heights of neutral brushes at different grafting densities. The value $b = 1.1$ delivered the closest agreement of simulation and SCF, and we henceforth suggest to stick to this value instead of the formerly applied value of $b = 1.3$.

The inaccuracy of the Kuhn length remained undetected because in Figure 4 (page 7849) and Figure 5 (page 7850) the salt concentrations of the MD simulations were incorrectly defined as the concentrations of salt ions instead of salt molecules. Below are the corrected versions of both pictures, in which we have used the more appropriate Kuhn length of $b = 1.1$ for the SCF calculations. The resulting density profiles display only minor differences from the previous ones, and all conclusions drawn from the original data remain valid.

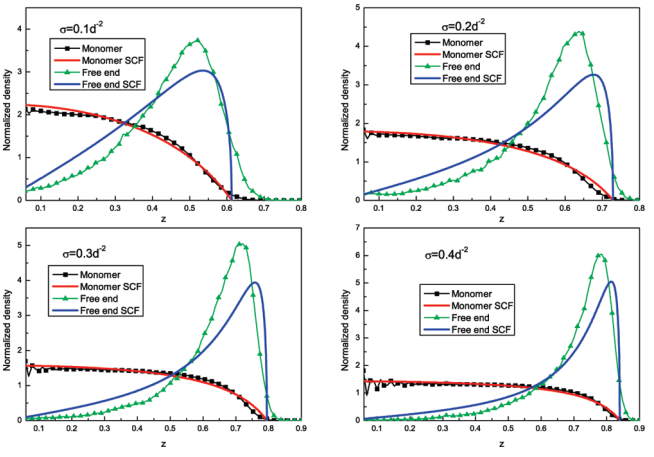

Figure 4. Monomer and end-monomer density profiles at different grafting densities σ. Here, the Bjerrum length was fixed to $l_B = 0.1d$ and the background salt concentration to $n_\infty = 0.13d^{-3}$.

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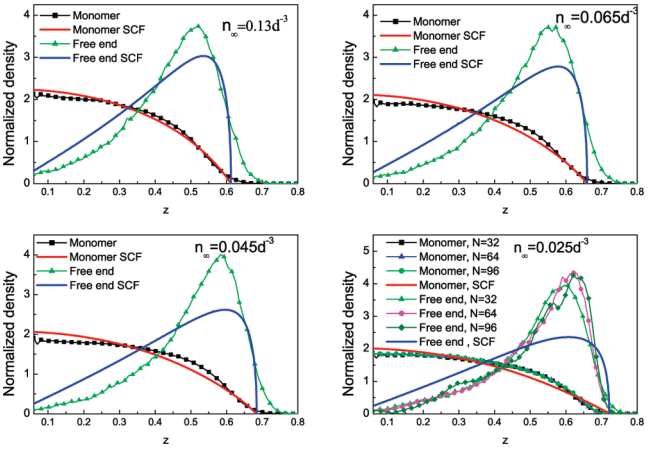

Figure 5. Monomer and end-monomer densities for various salt concentrations n_∞ and γ parameter as defined in eq 12. Simulations with low salt concentration ($n_\infty = 0.025d^{-3}$, lower right panel) were carried out with different chain lengths.