Monte Carlo Simulations of End-Adsorption of Head-to-Tail Reversibly Associated Polymers: Supplementary Materials

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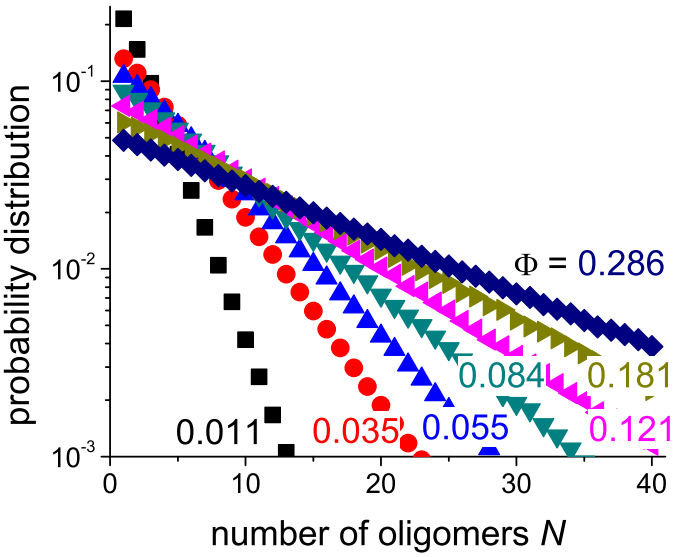
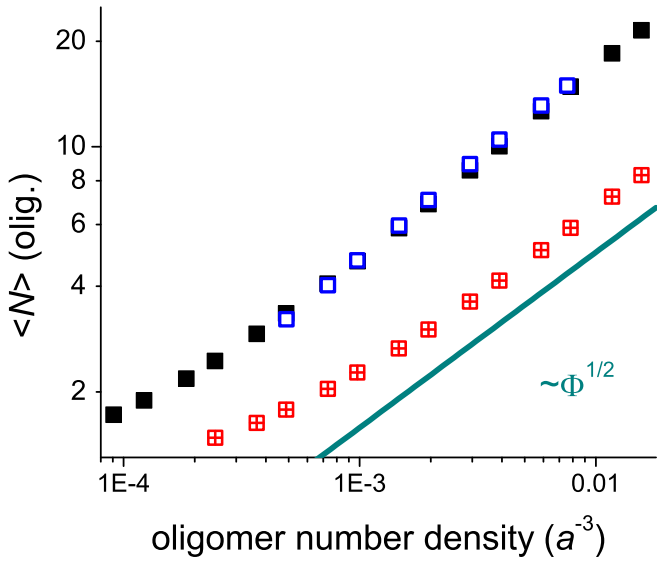
Bulk properties

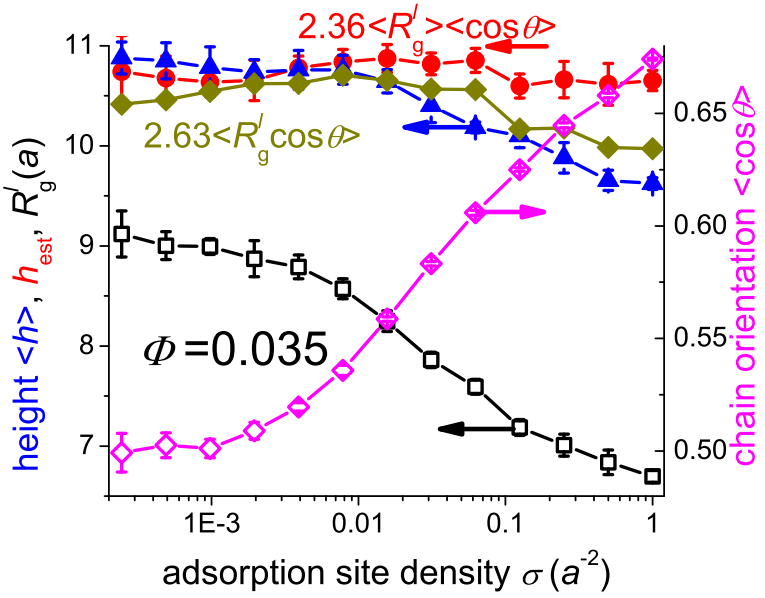


Chain length distribution for reversible associated polymers in the bulk for various polymer volume fractions Φ. Ring species are excluded from the calculation.

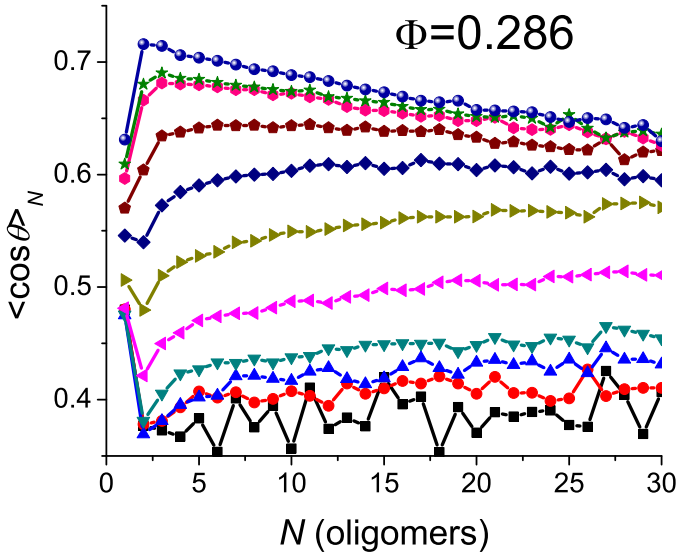


Average number of oligomers per chain as a function of oligomer number density (the total number of oligomers divided by the volume of the system). Solid (open) symbols are for the oligomer length 4 (8) and the energy of association $10kT$, crossed symbols are for the oligomer length 4 and the energy of association $8kT$.

Conformation of adsorbed chains



Average height of the adsorbed polymer layer (triangles) for the polymer bulk volume fraction $\Phi = 0.035$ as a function of adsorption site density in comparison with $h_{\rm est} = 2.36\ \langle R_{\rm g}^l \rangle \langle \cos\theta \rangle$ (circles) and $h_{\rm est} = 2.63\ \langle R_{\rm g}^l \cos\theta \rangle$ (dimonds). The long axis component of the radius of gyration $\langle R_{\rm g}^l \rangle$ is shown as open squares, whereas $\langle \cos\theta \rangle$ characterizing the chain orientation with respect to the surface normal is shown as open diamonds (right axis).



Average orientation $\langle \cos\theta \rangle$ of adsorbed polymer long axis with respect to the surface normal as a function of the number of oligomers in an adsorbed chain for different adsorption site densities ($\sigma = 2.44 \times 10^{-4} a^{-2}$ to $\sigma = 1 a^{-2}$ from bottom to top) for $\Phi = 0.286$.