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The effect of branching in modeling adsorption of impurities by polymeric adsorbents

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We consider a generalized lattice model describing adsorption of dispersed obstacles on a set of branched polymer structures. There is a strong experimental evidence that branched adsorbents could be essentially more efficient than their linear counterparts. We focus on two the simplest
representatives of the core-shell branched architectures: the star-like (with zero-dimensional point-like core) and comb-like polymers (with one-dimensional rigid core) with various number of branches, f, branch lengths, N, and branch separations, S (for the case of comb-like structure).
The quantitative estimates for adsorption capacity ⟨na⟩ in terms of adsorbed obstacles per monomer and the average number of bonds ⟨nbond⟩ per adsorbed obstacle (average adsorption strength) have been evaluated in a wide range of parameters f, N, and S. Both the case of implicit
diffusion of obstacles (with averaging over different arrangements of immobilized obstacles), and explicit diffusion of obstacles (allowing to study dynamics of adsorption process) have been analyzed. We found that comb-like polymers display the higher adsorption capacity but lower adsorption strength, comparing to the star-like polymers, and these effects are more pronounced with increasing branches separations S. Our analysis indicates essential role of bridging between adjacent branches by shared adsorbed particles.

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