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# Brownian dynamics simulation of model dendrimer adsorption by an attractive surface

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Brownian dynamics simulations were carried out for perfectly branched dendrimers of third generation, interacting with a structureless attractive surface. A freely jointed bead-rod model with excluded volume has been used. The dependence of conformational properties on the depth of potential well were obtained.

Методом броуновской динамики проведено моделирование процесса адсорбции модельного дендримера бесструктурной поверхностью. Использована модель свободно сочленённого дендримера с исключёнными объёмными взаимодействиями. Получена зависимость конформационных свойств дендримера от силы притяжения поверхности.

Dendrimers are macromolecules with tree-like architectures. The adsorption of dendrimers by an attractive surface is of significant interest in view of the possibility to create high-quality coatings of various types (see, e.g. [1]), consisting of dendrimer monolayers, as well as of promising biomedical applications of dendrimers in targeted drug delivery through the cell membrane (see, e.g. [2]). In the latter case, the conformational properties of denrimers, including different behavior of inner and outer segments during the adsorption process, are of especial importance, in due to the possibility of precise attachment of drug molecule to a specific site of the dendrimer [3].

In the previous papers, computer simulations of dendrimer's adsorption were performed by Monte-Carlo simulations in the frame of the lattice model [4–6]. The simulation within continuous model, performed in the present work, revealed new significant features of the adsorption processes, which don't manifest themselves within lattice model. For the Brownian dynamics study of the interaction of a third-generation dendrimer (shown schematically in Fig. 1) with a structureless surface, a freely jointed bead-rod model with excluded volume was used. The simulation details are similar to those described in [7]. A Lennard-Jones potential was employed for the surface-dendrimer interaction.

The dependences of all average values, characterizing the adsorption process, on the attractive potential well depth $\varepsilon$ (expressed in $kT$ units) reaches two plateaus at low $\varepsilon$ ($\varepsilon \leq 1$) and high $\varepsilon$ ($\varepsilon > 4$) $\varepsilon$ (see, e.g., Fig. 2). The region $1 < \varepsilon < 5$ corresponds to the transition of the dendrimer between the practically desorbed and completely adsorbed states.

The conformational behavior of the dendrimer, interacting with the attractive sur-