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非选择性溶剂中两嵌段共聚物的吸附及Scheutjens-Fleer理论与Monte Carlo模拟的比较

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摘要 Systematic comparison between computer simulation results and those predicted by Scheutjens-Fleer (SF) self-consistent-field theory is presented for the adsorption of diblock copolymers from a non-selective solvent on attractive surface. It is shown that although SF is a mean-field theory, it can qualitatively describe the adsorption phenomena of diblock copolymers. However, systematic discrepancy between the theory and simulation still exists. The approximations inherited in the mean-field theory such as random mixing inside a layer and the allowance of direct back folding may be responsible to those deviations.

关键词 Scheutjens-Fleer theory diblock copolymer surface adsorption Monte Carlo simulation

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Adsorption of Diblock Copolymers from Non-selective Solvent: Comparison Between Scheutjens -Fleer Theory and Monte Carlo Simulation

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Abstract Systematic comparison between computer simulation results and those predicted by Scheutjens-Fleer (SF) self-consistent-field theory is presented for the adsorption of diblock copolymers from a non-selective solvent on attractive surface. It is shown that although SF is a mean-field theory, it can qualitatively describe the adsorption phenomena of diblock copolymers. However, systematic discrepancy between the theory and simulation still exists. The approximations inherited in the mean-field theory such as random mixing inside a layer and the allowance of direct back folding may be responsible to those deviations.

Key words Scheutjens-Fleer theory; diblock copolymer; surface adsorption; Monte Carlo simulation

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