

热力学

非对称两嵌段高分子在选择性壁面识别吸附的Monte Carlo模拟

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摘要

采用自由空间的Monte Carlo (MC) 方法研究了两嵌段非对称高分子在选择性壁面上的吸附与识别。研究表明;非对称嵌段高分子同对称嵌段高分子一样;在选择性壁面的吸附可分为吸附和识别两个过程。对高分子构型研究的结果发现;无论条纹宽度如何变化;高分子在垂直于z方向的均方回转半径总是小于其垂直另两方向的值。在条纹宽度一定的情况下;尾式构型比率随链节B与白色条纹壁面作用能 $\Psi^{B-white}$ 增加先增加然后趋于不变。在 $\Psi^{B-white}$ 不变的情况下;尾式构型比率则随条纹数的增加而增加。环式构型比率在条纹较宽时会随 $\Psi^{B-white}$ 有一小的下降趋势;而在条纹较窄时下降幅度较大。

关键词

[非对称高分子](#) [识别](#) [选择性壁面](#) [Monte Carlo模拟](#)

分类号

Monte Carlo simulation of asymmetrical di-block copolymer adsorption and recognition at pattern surface

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Abstract

The adsorption of asymmetrical di-block copolymer on stripe-patterned surfaces has been investigated by off-lattice Monte Carlo (MC) simulation. The results showed that the polymer-surface binding of asymmetrical di-block copolymer was the same as symmetrical di-block copolymer proceeding in two steps; i.e., adsorption and recognition. With studies on the configuration of polymers; the mean-square radius of gyration along z axis was always smaller than that along x or y axis regardless of the width of stripes. It was shown that tails firstly increased and then kept unchanged with increasing adsorption energy when the width of stripes slit was fixed. When adsorption energy was fixed; tails increased with increasing number of stripes. Loops had a small trend to descend when the width of stripes was larger. But the downtrend of loops increased rapidly with narrower stripe width.

Key words

[asymmetrical copolymer](#) [recognition](#) [pattern surface](#) [Monte Carlo simulation](#)

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