Self-attracting self-avoiding trails on the triangular lattice interacting with a surface

Trabalho #15

> Apresentação Oral
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We investigate via extensive Monte Carlo simulations the phase behavior of self-avoiding trails defined on the triangular lattice, in the presence of a surface. In such system, independent two- and three-body on-site monomer-monomer interactions are considered, beyond a monomer-surface attraction, which are weighted by the parameters ω_2, ω_3 and κ, respectively. The tridimensional phase diagram of the system is featured by continuous and discontinuous transition surfaces among four phases: swollen (coil), globule, crystal and adsorbed. This last one always appears for large κ, but presents two distinct features depending on the other parameters: a phase (Ad$_1$) characteristic of an ordinary adsorption, where a single line is formed at surface in the ground state; and a phase (Ad$_2$) forming an adsorbed bilayer. Although some evidence of an Ad $_1$-Ad$_2$ transition exist in our data, a finite-size analysis indicates that there is only a crossover between them. For small κ, we find the crystal phase for large ω_3 and not so large ω_2, the globule phase for large ω_2, and the coil phase in a limited region of small ω_2 and ω_3. The phases coil-globule, coil-adsorbed, globule-crystal and globule-adsorbed are separated by surfaces of continuous transitions, while between the coil and crystal phases there is a coexistence (i.e., a discontinuous transition) surface. The crystal-adsorbed transition is discontinuous (continuous) for small (not so small) ω_2, with the associate surfaces meeting at a tricritical line. Beyond this line, we find also a line of critical-end-points, as well as three multicritical lines, where the transition surfaces above meet, yielding a very rich and interesting thermodynamic behavior.

Comentários adicionais

> Trabalho em processo de subimissão