Structural Characterization of Linear Three-Dimensional Random Chains: Energetic Behaviour and Anisotropy

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Abstract

In this work, we will make an energetic and structural characterization of three-dimensional linear chains generated from a simple self-avoiding random walk process in a finite time, without boundary conditions, without the need to explore all possible configurations. From the analysis of the energy balance between the terms of interaction and bending (or correlation), it is shown that the chains, during their growth process, initially tend to form clusters, leading to an increase in their interaction and bending energies. Larger chains tend to “escape” from the cluster when they reach a number of “steps” $N>\sim 1040$, resulting in a decrease in their interaction energy, however, maintaining the same behavior as flexion energy or correlation. This behavior of the bending term in the energy allows distinguishing chains with the same interaction energy that present different structures. As a complement to the energy analysis, we carry out a study based on the moments of inertia of the chains and their radius of gyration. The results show that the formation of clusters separated by “tails” leads to a final “prolate” structure for this type of chain, the same structure evident in real polymeric linear chains in a good solvent.

Keywords

Self-avoiding random walk, Linear chains, Interaction energy, Bending energy, Moment of inertia, Radius of gyration, Asphericity, Prolate structure