

Ground-state properties of thick flexible polymers

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We investigate ground-state properties of a simple model for flexible polymers, where the steric influence of monomeric side-chains is effectively introduced by a thickness constraint [1]. Thickness is defined via the global radius of curvature [2]. From parallel tempering and flat-histogram computer simulations, we find a strong thickness dependence of the conformational topology of the ground-state structures. A systematic analysis for short polymers allows for a thickness-dependent classification of the dominant ground-state topologies. It turns out that helical structures, strands, rings, and coils are natural, intrinsic geometries of such linelike objects.

[1] T. Neuhaus, O. Zimmermann, and U.H.E. Hansmann, *Phys. Rev. E* **75**, 051 803 (2007).

[2] O. Gonzalez and J. Maddocks, *Proc. Natl. Acad. Sci. USA* **96**, 4769 (1999).