

Meeting: 1002, Pittsburgh, Pennsylvania, SS 7A, Special Session on Knots and Macromolecules

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Topological Properties of Polymer Chains: The Influence of Model. Preliminary report.

Different models of polymer chains are used in computations of their topological properties. We investigated how these properties depend on the chain model. To study the issue we calculated the probability to form a nontrivial knot for different models. We compare different freely jointed and the wormlike chain models. The computations showed that different models predict not only different absolute values of the probabilities but also different scaling properties. We also performed comparison for different ways of incorporating the excluded volume effect into a model chain. It was found that the models of hard cylinders and hard spheres with the same values of the second virial coefficient of the chain segments predict different values of the knotting probabilities. (Received September 11, 2004)