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The influence of topology on the free energy and metric properties of ring polymer confined in a slit¹ ZHAO-YAN SUN, BING LI, LI-JIAN AN, ZHEN-GANG WANG, None — An off-lattice model with no excluded volume is used to study the effect of topological constraint on the free energy and metric properties of ring polymer confined in a slit with height d . The topological state is conserved by forbidding bond crossing. This model was applied to ring polymers with chain length up to $N = 10^3$. Umbrella sampling and weighted histogram analysis method (WHAM) are used to calculate the free energy and the radius of gyration. In the strong confinement limit, free energy of linear chain in our model scales as d^{-2} and the in-plane radius of gyration $R_{||}$ is independent of confinement, which agrees with the theoretical prediction very well. However, unlike the linear chain, the scaling behavior of ring polymer shows a different trend. This abnormal scaling behavior is thought to be caused by the topological constraint: the knotting probability of ring polymer increases with decreasing the slit height, and in this case, ring polymer is forced to expand itself to conserve its topological unknotted state.

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