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(U*) Simulation of Two Polymers Confined to a Box-Like Cavity: The Effect of Anisotropies in Polymer Length and Confinement Dimensions

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The behaviour of confined polymeric systems has been the topic of much recent research. The information from these studies may help guide the development and optimization of nanofluidic devices and understand the segregation of DNA chromosomes in prokaryotic cells. Some recent experiments examined two DNA molecules confined to a box-like cavity with strong confinement in one dimension. The researchers looked at the effect of using an anisotropic cross-sectional box geometry and of having non-identical polymers. In this study, we use computer simulations to examine the effect of such anisotropies on the behaviour of the confined-polymer systems. We employ Metropolis Monte Carlo simulations where the polymers are modelled as bead spring chains. We calculate probability distributions for the centre-of-mass positions of either polymer and for the centre-of-mass displacement between the polymers. These distributions are used to examine the effect of anisotropies in polymer length for two polymers confined to a square box-like cavity and anisotropies in box dimensions for two identical polymers confined to a box-like cavity. The information obtained from this study can then be used to have a better understanding of the trends seen in the experiments.

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