

Abstract Submitted
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Effect of Nanopore Confinement on the Polymerization Rate of Linear Polymers PO-HAN LIN, RAJESH KHARE, Texas Tech University — Confinement to a nanopore has a significant impact on the thermal properties as well as the rate of chemical reactions such as polymerization as compared to these processes in the bulk. In this work, we have studied the effect of nanopore confinement on the rate of free radical polymerization by using molecular simulations. In order to capture the physics of this process, we have implemented a coarse-grained model to carry out reactive molecular dynamics simulations. Our simulation method considers the three stages of polymerization process: initiation, propagation and termination. Our simulation results will be used to compare the polymerization rate in the confinement with that in the bulk. The results will be explained by focusing on the dynamics of the reacting species in the confinement.

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