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Title:	Molecular Dynamics Simulation of Unzipping of a Polymer Hairpin by Force
Authors:	Rani, Jyoti (/jspui/browse?type=author&value=Rani%2C+Jyoti)
Keywords:	Physics Dynamics Polymer
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Abstract:	Polymers have universal behaviour at long time scales and at long length scales. Large scale molecular dynamics simulations were carried out to study the structural properties of polymers. Specifically the dependence of chain length, also the excluded volume effect was introduced. For a linear polymer of chainlength $N = 128$ a good agreement was found with the size exponent. The model was extended to the hairpin configuration. The polymer hairpin unzipping has been studied via equilibrium force- induced unzipping and temperature-induced unzipping. The force-induced unzipping showed a first order phase transition. While the temperature-induced unzipping is found to be continuous phase transition.
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