

Size-effects in Polymer Stretching

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Stretching of small polymer segments, like mRNA, have properties depending on the size and shape of the polymer. In this work, with computer simulations, we have studied the different stretching properties of short polymer segments, varying from 5 to nucleotides (with variations of different nucleotides), in addition to two structures (1ZIG and 2KOC). The stretching is done with either isotensional or isometric stretching, i.e., we either control the force or the distance between the two terminal ends of the polymer.

From this work we can find a substantial finite-size effect between the different polymer segments. We compute the Gibbs- and Helmholtz energy for the stretching process and compute the different degrees of stacking during the stretching. Stretching these segments is found to be irreversible on the short timescale, and the orientation of the nucleotides helps stabilize the structures. During a relaxation step, the old structure is not recovered.

The stability of short polymer strains is dependent on the size and composition of these strains. We find the whole process to be a non-equilibrium process, where the initial structure is not recovered in the timescales accessible in the simulation. We believe a better understanding of these processes can help understand the folding and un-folding of biopolymers during normal cell function.