1004-92-236 **Alexander Vologodskii\*** (`alex.vologodskii@nyu.edu`), Deparment of Chemistry, New York University, 31 Washington Place, New York, NY 10003, and **Anatoly Borovik**. *Diffusion of knots along stretched DNA molecule.* Preliminary report.

Brownian dynamics simulation is a generally accepted method for the modeling of motion in DNA molecule. This method allows nearly all the essential conformation changes in molecules of a few thousand base pairs in length to be addressed. Although this simulation of motion is well developed, it has not been critically tested because of a lack of experimental data on the internal motion of DNA. The recent work of Steve Quake and co-workers, who were able to tie individual DNA strands into knots, has produced a data set of this kind, however. After the knots were formed the DNA molecules were stretched by optical tweezers and the knots then became highly localized. The group observed diffusion o f the knots along stretched DNA and measured the diffusion coefficients for the five simplest knots. We simulated the knot diffusion on the stretched DNA by Brownian dynamics, using a well developed bead model of the double helix. These results were compared with the experimental data. (Received January 25, 2005)