Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Kinetic simulations of tension-induced DNA strand-unpeeling transition YUANYUAN QU, Department of Physics, National University of Singapore, HONGXIA FU, Mechanobiology Institute, Singapre, National University of Singapore, JIE YAN, Mechanobiology Institute, Singapore, Department of Physcis, National University of Singapore — Sequence- and salt- dependent kinetic simulation assuming strand-unpeeling from B-DNA using the Gellispie's stochastic kinetics simulation algorism was performed for DNA fragments of a few hundred base pairs. Similar to DNA unzipping experiments, sequence-dependent energy barriers resulted stepwise extension changes were observed during the transition. The simulations were compared with recent single-molecule studies of overstretching transition of the same DNAs occurring at around 65 pN. The results quantitatively reproduced the dynamics of overstretching transition of the same DNAs under conditions when overstretching led to strand separation, and were distinct from that when the transition led to a double-stranded overstretched DNA called "S-DNA" through the B-S transition pathway. We conclude that the strand separation transition pathway was a strand-unpeeling transition from the two free ends of DNA. Further, our results suggest that the B-S transition pathway does not involve base-pair separation.

Yuanyuan Qu
Department of Physics, National University of Singapore

Date submitted: 17 Nov 2010 Electronic form version 1.4