Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Computer simulations of polymer reversal inside a pore LEI HUANG, DMITRII E. MAKAROV, University of Texas at Austin — Translocation of biopolymers through pores is implicated in many biological phenomena. Confinement within pores often breaks ergodicity on biological time scales by creating large entropic barriers to rearrangements of the chain. We study one example of such hindered rearrangement, in which the chain reverses its direction inside a long pore. Our goal is two-fold. First, we study the dependence of the polymer reversal timescale on the pore size and on the polymer length. Second, we examine the ability of simple theories, such as transition state theory (TST) and Kramers' theory to quantitatively describe a transition in a system with a complex energy landscape. We find that one-dimensional TST using the polymer extension along the pore axis as the reaction coordinate adequately accounts for the exponentially strong dependence of the reversal rate on the pore radius $r$and the polymer length N, while the transmission factor, i.e., the ratio of the exact rate and the TST one, has a much weaker, power law r and N dependence.

Lei Huang
University of Texas at Austin

Date submitted: 26 Nov 2007 Electronic form version 1.4