Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Non-Equilibrium Dynamics of Nano-channel Confined DNA: A Brownian Dynamics Simulation Study ANIKET BHATTACHARYA, AIQUN HUANG, University of Central Florida, WALTER REISNER, McGill University, Canada — We carry out Brownian dynamics (BD) simulation for a semi-flexible polymer chain characterized by a contour length Na and a persistence length ℓ_p confined inside a rectangular nanochannel to study its compression and retraction dynamics while being pushed on one end at a constant velocity by a "nano-dozer". We study the evolution of one dimensional concentration profile $c(x,t)$ and the chain extension R along the channel axis (x-axis) during both the contracting as well as the retracting phases as a function of the velocity of the nano-dozer, both in steady states and in transients. Furthermore, we measure the transverse fluctuations of the chain under contraction and retraction, and the amplitude of the density profile, and compare these simulation results with those obtained from an analytical model proposed by Khorshid *et al.* Our studies are guided by recent experimental results by Khorshid *et al.* (Phys. Rev. Lett, **113**, 268104 (2014)) and provide further justification to use a one dimensional PDE approach to understand the non-equilibrium dynamics of confined polymers.

Aniket Bhattacharya
University of Central Florida

Date submitted: 05 Nov 2015 Electronic form version 1.4