Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Thermophoretic Regulation of Molecular Flux through a Nanopore[1] MAXIM BELKIN, ALEKSEI AKSIMENTIEV, University of Illinois at Urbana-Champaign — Transport of ions, nucleic acids and other molecular species through pores in thin membranes is a process of fundamental importance to the biological function of a cell and practical applications in the field of molecular separation, filtering, and, recently, DNA sequencing. Various approaches to control the transport have been examined, including the effects of the geometry, charge and chemical functionalization of the nanopore surface. Thermophoresis in liquids, i.e. movement of molecules along a temperature gradient, was discovered more than a century ago and has already been employed in various applications, typically involving macroscopic systems. In this work, we explore the use of thermal gradients for regulation of nanoscale fluxes. Specifically, we use all-atom molecular dynamics simulations to examine the effect of thermal gradients on transport of ions, small organic solutes and long DNA molecules through solid-state nanopores. In our typical simulation, multiple thermostats are applied to different parts of the same simulation system, allowing steady-state temperature gradients to be established and the effective forces associated with the thermal gradients to be determined. The results of our simulations suggest that nanopore fluxes of molecular species can be regulated by means of thermal gradients. We expect our results to find applications in molecular separation and filtering technologies, nanofluidic electronics and nanopore sequencing of DNA.

[1]This work was supported through NSF DMR-0955959

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Date submitted: 09 Nov 2012 Electronic form version 1.4