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Origin of translocation barriers for polyelectrolyte chains RAJEEV KUMAR, Materials Research Lab, UCSB, CA, MURUGAPPAN MUTHUKUMAR, University of Massachusetts, Amherst, MA — For single-file translocations of a charged macromolecule through a narrow pore, the crucial step of arrival of an end at the pore suffers from free energy barriers, arising from changes in intrachain electrostatic interaction, distribution of ionic clouds and solvent molecules, and conformational entropy of the chain. All contributing factors to the barrier in the initial stage of translocation are evaluated by using the self-consistent field theory for the polyelectrolyte and the coupled Poisson-Boltzmann description for ions, without radial symmetry. The barrier is found to be essentially entropic, due to conformational changes. For moderate and high salt concentrations, the barriers for the polyelectrolyte chain are quantitatively equivalent to that of uncharged self-avoiding walks. Electrostatic effects are shown to increase the free energy barriers, but only slightly. The degree of ionization, electrostatic interaction strength, decreasing salt concentration and the solvent quality all result in increases in the barrier.

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