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Ion distribution inside a nanopore in the presence of a polyelectrolyte LEI GUO, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — Experimental studies of the translocation of DNA through nanopores rely on measurements of the ionic current. In order to understand the behavior of this current, we employ molecular dynamics simulations to study the ion distribution within a nanopore in the presence of a polyelectrolyte. We characterize the ion distribution in terms of radial density profiles around the polyelectrolyte. Several factors affecting the ion distribution are studied, including the role of chain flexibility, salt concentration, nanopore size and its polarizability. Our study also provides information on the dynamics of the ions inside the pore. The combination of static and dynamic information is used to explain experimental observations.

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