

Ion transport and selectivity in nanopores with spatially inhomogeneous fixed charge distributions

Ramírez P, Gómez V, Cervera J, Schiedt B, Mafé S

JOURNAL OF CHEMICAL PHYSICS 126 (2007) 194703

Polymeric nanopores with fixed charges show ionic selectivity when immersed in aqueous electrolyte solutions. The understanding of the electrical interaction between these charges and the mobile ions confined in the inside nanopore solution is the key issue in the design of potential applications. The authors have theoretically described the effects that spatially inhomogeneous fixed charge distributions exert on the ionic transport and selectivity properties of the nanopore. A comprehensive set of one-dimensional distributions including the skin, core, cluster, and asymmetric cases are analyzed on the basis of the Nernst-Planck equations. Current-voltage curves, nanopore potentials, and transport numbers are calculated for the above distributions and compared with those obtained for a homogeneously charged nanopore with the same average fixed charge concentration. The authors have discussed if an appropriate design of the spatial fixed charge inhomogeneity can lead to an enhancement of the transport and selectivity with respect to the homogeneous nanopore case. Finally, they have compared the theoretical predictions with relevant experimental data.