CECE 2017

CECE 2017

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Abstract

For nanopores, there can be made a difference between natural and artificial nanopores, as ion channels and carbon nanotubes or nanopores cauterized into foils. Artificial nanopores have microscopic-length and a nanoscopic radius-size. Ion transport through the nanopore is connected with an important property: the selectivity. Due to this property the nanopore can be used, for instance, as a nanoscopic porus sensor.

The basic concept of our model nanopore sensor is that the presence of an analyte molecule modulates the ionic current flowing through the pore. The analyte molecule (usually a biomolecule) is detected selectively if it is bound to the nanopore. If the binding is a reversible process involving physical forces that are weaker than chemical bonds, the probability that the analyte molecule binds to the nanopore is proportional to its concentration. From calibration curves (current vs. concentration) the analyte concentration can be determined.

In this modeling work, we create simple models the membrane, the pore and the electrolyte. Negative charges are located on the cylindrical pore's wall to make the pore cation selective. For the electrolyte, the Primitive Model of electrolytes is used, which treats the ions as hard spheres with their charges located in the centers, and the solvent as a constant dielectric continuum. The binding sites are modeled with a square-well potential. We applied the Local Equilibrium Monte Carlo (LEMC) method coupled with Nernst-Planck (NP) equation. This method (NP+LEMC) is suitable for study even micromolar concentrations.

We present a modeling study to analyze the device sensitivity (defined as I/I0, where I and I0 are the currents in the presence and absence of the analyte, respectively) to the various model parameters: number, strength, and width of the binding sites; properties of the electrolyte and the analyte. Through the calculated concentration profiles, the molecular mechanisms of the system can be understood.