Molecular Dynamics Study of the Ion Transport in Porelike Protein Channels

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In many cases the ion transport through biological membranes takes place via pore-like protein channels. The elementary process of this transport can be described as the motion of the ion in a quasi-periodic multi well potential.
In this study molecular dynamics simulations of the ion transport in a model pore were performed to test the validity of the elementary reaction rate theory for this process. We have chosen a hexagonal helix with periodical boundary conditions as a model pore. In this model the potential energy for the ion as a function of the migration coordinate results from Coulomb-interactions between the ion and polar groups located at the surface of the helix. The polar groups were represented by oscillating dipoles coupled by dipole-dipole interaction. Thirty dipoles were used per unit cell. The classical equations of motion for the ion and the dipoles were solved simultanously with the aid of a numerical integration procedure. In this calculation it was possible to thermalize the system of dipoles,so that the ion diffusion could be studied as a function of temperature.
It could be demonstrated, that the diffusion rate for the ion is sensitively dependent on the equilibrium orientation of the dipoles. For parallel orientation the ion can migrate nearly free along the helix axis while if the dipole orientation alternates along the helix chain the ion migrates according to a jump mechanism and the temperature dependence of the ion diffusion coefficient can be described by an Arrhenius like behaviour. In this latter case, the activation energy roughly agrees with the static energy barrier between the potential wells, but the preexponential factor does not depend on the temperature.

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