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Morphometric approach to selectivity and gating of ion channels
ROLAND ROTH, MPI fuer Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany — A physical understanding of selectivity and gating of ion channels requires the free energy of the fluid confined in the channel pore. The free energy depends not only on fluid properties like its density, but also on the interaction between fluid particles and the confining protein, which gives rise to a potentially complicated dependence of the free energy on the conformation of the protein. Here we propose a simple thermodynamic approach that employs the idea that the free energy can be separated into geometrical measures and corresponding thermodynamic coefficients. Our approach enables us to calculate the change in the free energy caused by a change of the pore conformation such as that underlying the gating of an ion channel. We study the connection between the geometrical change of a hydrophobic pore and capillary evaporation, i.e. the effect that water is expelled from the permeation pathway and ion flow is thereby stopped although the pore remains wider than the water or ion diameters. We estimate the energy it takes to remove the water from the pore. Within the same thermodynamic framework, we can also study effects of pore conformation on the equilibrium absorption of ions and thus on ionic selectivity of the channel.

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