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Ion Channels as Nanodevices

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Ion channels are proteins surrounding a hole that allow substances to cross biological membranes. The concentration or current of these substances controls an enormous range of biological function: ion channels are nearly as important in biology as transistors in computers. Ion channels have a stable structure (on biological time scales $> 0.1\mu$sec) once open and so current through them can be analyzed by 'physics as usual'. The permanent charge on the wall of the channel is large and the volume is tiny, so the number density of ions in the channel is very large, >10 M. Physical properties of channels can be understood from the balance between electrical and van der Waals forces of charge crowded into a tiny space. Many biological properties of channels can be understood in the engineering tradition of devices: channels follow reasonably robust 'device equations' determined by their specific structural design and general physical environment. Channel research seeks to understand these device equations in ***just*** enough detail to control them. Channels—like most engineering devices—function away from equilibrium, so spatially non-uniform boundary conditions and non-equilibrium statistical mechanics must be used in their description. Atomic scale simulations pose certain problems since trace concentrations of ions ($< \mu$M) often control biological function and ions flow on time scales very much slower than the time steps of simulations. Atomic scale simulations of microM activities requires enormous numbers of water molecules ($>10^{11}$); direct simulation of ionic current involves many billions ($>10^{11}$) of time steps, suggesting that analysis must be multiscale if it is to be useful. This should come as no surprise, since the function of ion channels is inherently multiscale: ion channels act as nanovalves, nanodevices that allow details of atomic structure to control macroscopic flows and biological function.

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