

Molecular pumps and motors in biology

Gerhard Hummer

*Department of Theoretical Biophysics, Max Planck Institute of Biophysics,
Frankfurt am Main, Germany*

Biomolecular machines carry out a wide range of functions, from chemical sensing and signaling over highly selective molecular transport to the efficient interconversion of chemical, mechanical, electrical, and light energy. We have used statistical mechanical theory and molecular dynamics simulations to characterize the molecular mechanisms underlying some of these biological processes. Remarkably, common physical principles emerge in the function of proteins serving as proton pumps, transporters, and molecular motors, despite large variations in their structure and biological role. In particular, water and hydration effects coupled to protein motions occupy central roles in the operation of these molecular machines, and are key to achieving both high efficiency and high fidelity.