

Physical models of mitochondrial proton-pumping complexes

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A proton gradient across a lipid membrane is a common intermediate form of energy storage in biological systems, which is subsequently converted into a proton current and, finally, into the most stable energy of chemical compounds. Even in a single physical system, the inner mitochondrion membrane, there is a variety of mechanisms pumping protons across the membrane, therefore converting the energy of high-energetic electrons into the proton gradient. With the molecular structures of the proton-pumping Complexes I, II, and IV being resolved in detail, actual physical mechanisms of the energy conversion often remain elusive. In this presentation, I will discuss our old and very recent results in modeling the proton-pumping complexes. In Complex IV, the energy transfer due to the direct electrostatic interaction occurs when the electrons and protons populate the sites in close proximity. In Complex I, where the electron and proton sites are well separated, it is assisted by conformational changes in the protein environment. In Complex III, the energy is transferred by means of the electron-proton interaction on the quinone shuttle. In our quantitative approach, we wrote the Heisenberg equations of motion for the electron and proton operators in the presence of the protein environment. In the high-temperature limit, they can be rewritten as the rate equations for the electron and proton populations with the transfer matrix elements having a Marcus-like form. For Complex I, the rate equations are coupled with the phenomenological Langevin equation describing the dynamics of the conformational changes. For Complex III, the mechanical motion of quinones is also described by the Langevin equations. The obtained equations were solved numerically, and it was shown that the protons can be effectively pumped across the membrane within the proposed models for all the Complexes. Moreover, we demonstrated that for the actual sets of parameters, the proton pumping is the most efficient for physiological temperatures.