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über

Describing Charge Transfer in Proteins: A Microstate Model for Simple Proteins and Complex Machineries

Electron transfer plays a central role in many biological processes such as, for instance, photosynthesis or oxidative phosphorylation, but also in other bioenergetic processes such as denitrification or sulfate and sulfite reduction. Moreover, electron transfer is a key step in many enzymatic reactions. The framework of Marcus theory provides the theoretical basis to describe the kinetics of these reactions. The parameters to calculate rate constants can be estimated using protein crystal structures. Namely, the electronic coupling is related to the edge-to-edge distance between the redox-active sites. The reaction free energy and the reorganization energy can be obtained for instance from continuum electrostatic calculations. However, to perform complicated tasks, proteins often combine many redox cofactors and couple the redox reactions to protonation reactions or conformational changes. Moreover, electron transfer proteins are often embedded in membranes, and thus membrane potential and concentration gradients influence the reactions. One approach to describe such complex systems is the so-called microstate model, in which each state of a system is represented by a vector in which each component defines the status of each site (for instance oxidized or reduced, protonation or deprotonated). On the basis of this microstate description, it is possible to calculate the thermodynamics and kinetics of a complex protein system. In this article, we will review the principle features of the microstate model and explain how the parameters of the microstate model can be calculated using continuum electrostatics. The microstate model provides the theoretical framework to go from molecular structures to the mechanism of complex protein machines.

G. Matthias Ullmann, Lars Mueller, and Elisa Bombarda. Theoretical Analysis of Electron Transfer in Proteins: From Simple Proteins to Complex Machineries. In *Advances in Photosynthesis and Respiration Vol. 41: Cytochromes and Cytochrome Complexes: Structure and Function*. (William A. Cramer and Toivo Kallas eds), Springer Verlag. pp.99-127, 2016