Microscopic modeling of charge transport in sensing proteins

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Sensing proteins (receptors) are very intriguing materials. From one hand, they are quite small structures (about 5 nm diameter) and exhibit very complex behaviors (they can “pump” ions, use energy from the environment, change their shape, catalyze some reactions, etc). From another hand, they control the life of any organism at a cellular level. All of them are constituted by a specific sequence (several hundreds) of amino-acids (primary structure) and in this sequence the space organization (tertiary structure) is codified. Functioning of these macromolecules is intrinsically connected to their tertiary structure, and modifications in the former induce modifications in the latter; the reverse also happens. Most of protein receptors operate with a lock-and-key mechanism [1]. They possess an active site (lock) in which only few specific molecules (keys) can be attached. For some of them the specialization is so high that only one key is accepted, for example a photon. The key produces relevant modifications of the tertiary structure, which, in turn, are responsible for the protein functioning in the living system.

With the advance of nanotechnology, the investigation of the electrical properties of sensing proteins has emerged as a demanding issue. Beside the fundamental interest, the possibility to exploit the electrical properties for the development of bio-electronic devices of new generations has attracted major interest of many researchers. From the experimental side we cite three significant experimental approaches: (i) current voltage (I-V) measurements in nanometric layers of a given protein sandwiched between macroscopic (mm^2) contacts, (ii) I-V measurements within an AFM environment in nanometic monolayers of a given protein deposited on a conducting substrate, (iii) electrochemical impedance spectroscopy (EIS) on appropriate monolayers of self-assembled samples of a given protein. From a theoretical side, a microscopic interpretation of these experiments is still a challenging issue.

The aim of this talk is to address the above issue by reviewing recent theoretical results carried out by the Authors within an Euroean project,BOND (Biosensor 0lfactory Neuron Devices) [2], which provide a first quantitative interpretation of the three kinds of charge transfer experiments detailed above.

As significant examples, Figs. 1 and 2 compare different sets of experiments carried out on bacteriorhodopsin (a light receptor) and rat I7 (an olfactory receptor) with the corresponding theoretical modeling, showing the reasonable good agreement obtained. Details of the model as well as the potential applications of this research will be addressed at the Conference.

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References

[1] The lock-and-key theory is very old, it was revised in 1958 by D.E. Koshland Jr in the paper: *Application of a theory of enzyme specificity to protein synthesis,* PNAS 44, 98-104 (1958).

[2] More information on the project can be found at the web site: http://bondproject.org/. See also: E. Alfinito, C. Pennetta, L. Reggiani, *First evidences supporting the realization of smell nanobiosensors based on olfactory…*Sensors and Actuators B: Chemical, 146 , 554-558 (2010); E. Alfinito, J.-F. Millithaler, C. Pennetta, L. Reggiani, *A single protein based nanobiosensor for odorant recognition*, Microelectr. Journal. 41, 718 (2010).

[3] E. Alfinito, L. Reggiani, *Charge transport in bacteriorhodopsin monolayers:…,* Europhys. Lett. 85. 6802(1-6) (2009).

Figures

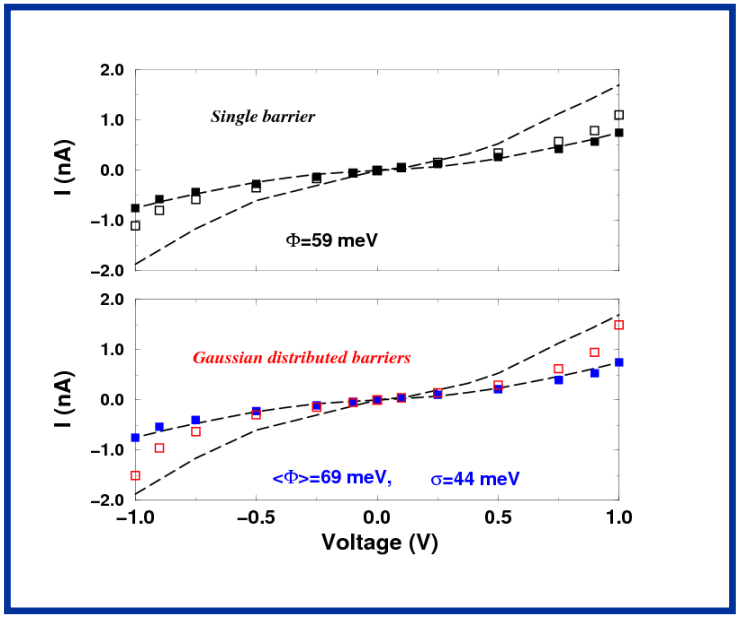

Figure 1. I-V characteristics for the native and activated state of bacteriorhodopsin [3]. Calculations (symbols) have been performed using a tunneling mechanism for charge transfer with a single value of barrier height (upper part of figure) and with a Gaussian distributed set of heights (lower part of figure. In both the cases the full squares refer to the native state, while the empty squares refer to the activated state. Dashed curves refer to experiments, the lower for the native state (in dark) the higher for the activated state (in the presence of a green light).

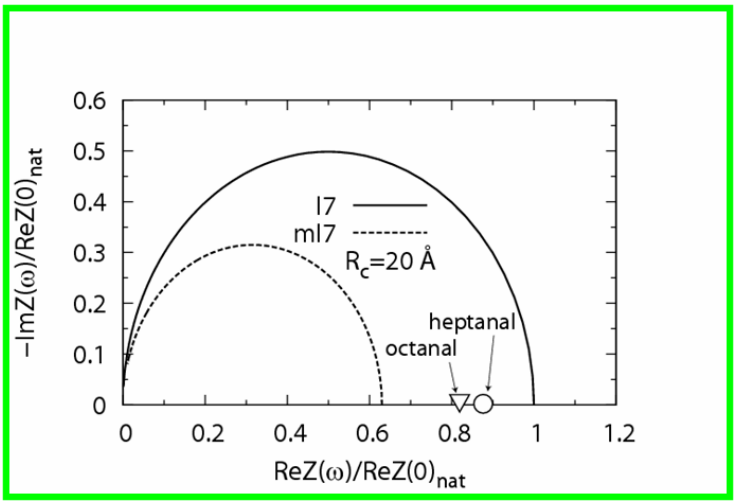

Figure 2. Nyquist plots for the native and activated states of the rat olfactory receptor I7 [3]. The continuous line reports the calculations for the native state, and the dashed line for the activated state when choosing an interacting radius between aminoacids of 20 A. The experimental resolutions obtained with an odorant concentration of 10^{-4} M for the two specific ligands, octanal and heptanal, are pointed out by the arrows