MODELS OF EXTENDED ELECTRON STATES IN PROTEINS

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The paper presents a new approach to study the electron states in complex biomolecular systems. We discuss their possible realization and the properties of extended electron states. By an extended electron state we mean a state which spreads over to tens and more atoms of the medium. The basis for their use in a condensed medium with a complex profile potential energy (biomacromolecule) may be a polaron model.

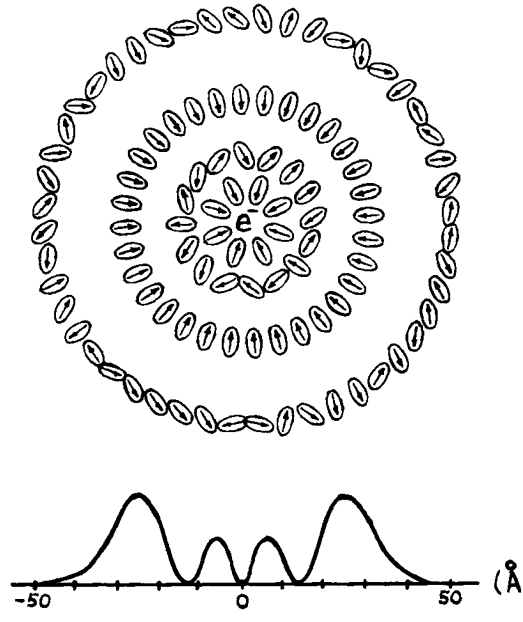

Fig. 1. The excited self-consistent state in a polar liquid. The arrows show dipole moments of the medium molecules. Below the density of medium polarization is plotted.

Molecular Electronics and Biocomputers.
Пущино: НЦБИ АН СССР, 1989.

It has been already shown /1,2/ that isotropic polar media may exhibit self-consistent polaron states of large effective radii (Fig.1).

We calculated the energy of the ground and the excited polaron states for the simplest model of a protein globule /3,4/, which is the model of a dielectric cavity. We obtained the estimates for polaron absorption and emission bands an example was cytochrome C_{559}. It has been found that the emission band of the excited polaron in a protein macromolecule is in the IR area and can be identified as assessing its impact on the factors like PH, ion strength, temperature etc. The results may be use to create a consistent theory of electron transfer in photoexcited macromolecules.

Literature

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