DIELECTRIC PROPERTIES OF FULLEREN- MODIFIED BILAYER LIPID MEMBRANES

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Abstract

The strong electron affinity of C_{60} makes it a good electron acceptor. It is capable of taking up several electrons as was shown by electrochemical measurements in organic solvents. When bilayer lipid membranes (BLM)modified by fullerenes, latter cathches electrons initially localized on lipid molecule bonds. A charged fullerene or complex of charged fullerenes - vacancy can be considered as the system which has a dipole moment. A polarization phenomenon is the key step in deep understanding of physical processes responsible for electrophysical and dielectric properties of lipid bilayers. Analytical solutions to average polarization of the fullerene molecules as well as energy and electron wave function of the excited p- state of the fullerenes were presented.

The growing interest in membrane technologies and in membrane processes is a strong incitement for the evaluation of the dielectric properties of fulleren modified bilayer lipid membranes [1-5], Lipid bilayers, the basis of natural membranes, are highly dynamic, two-dimensional, ordered systems. They provide simplified systems to study the complex biological membranes and the processes that are occurring therein. Also, these quasi two-dimensional, partially ordered structures with their unique elastic properties have led to a number of applications in biomedical devices: biocompatibilization of surfaces, drug delivery. Due to the easy way of their producing and stability on the surface of electrodes, the planar lipid bilayers (BLM) find new applications as biosensors and bioelectronic devices. [6].

In most of cases studies in this field include the introduction of organic molecules in the membranes in order to affect the permeability as well as the physical and mechanical properties of the current system. In this context, C_{60} fullerene have been introduced in lipid bilayers and their ability as both photosensitizers for electron transfer from donor molecules, and mediators for electron transport across the lipid bilayer have been studied [9-14]. The intercalation of C_{60} fullerene molecules inside a lipid bilayer may affect the motions and flexibility of the whole structure thus giving rise to new outstanding material properties. The strong electron affinity of C_{60} makes it a good electron acceptor. It is capable of taking up several electrons as was shown by electrochemical measurements in organic solvents [15-19] At present it is established that several types of impurities in lipid bilayers essentially influence on charge transfer processes. This allows to vary purposeful several properties of lipid bilayers at the doping and hence to improve sensibility of membrane-based biosensors. At the same time the fullerenes are distinguished with especial efficiency and doping BLMs by them increases efficiency of charge transfer through lipid bilayers and also affects on their dielectric properties. When BLM's doped by fullerenes, latter acquired an acceptor properties. Catching electrons initially localized on lipid molecule bonds, fullerenes acquire a negative charge. At the same time a charged fullerene or complex of charged fullerenes - vacancy can be considered as the system (quasydipole) which has a dipole moment. It is necessary to note that lipi d molecule has their dipole moment. Dipole-dipole interaction between the lipid molecules and formed quasydipoles and interaction of quasydipoles between one another lead to change of local electric field. Which thus depends on fullerene concentration in lipid bilayers and their capability of electron catching from valent bonds of lipid molecules.

Thus in this work we will consider dielectric properties of fulleren modified BLM's. In this report we will present analytical results for the average magnitude of the dipole moment of fulleren placed between two charged plates.

Potential of electrons in fullerenes we can describe on following:

$V(r) = V_0\delta(r-R)$ $V_0 = \kappa(1+ctg(\kappa R))/2$ and R=6.639 - is a fullerene radius. κ determines by $I_0 = 2.65eV = 0.195 = \kappa^2/2$. Here I_0 is the ionization potential od fullerene. $C_60's$ ground state wave function is:

$\psi = \frac{u(r)}{4\sqrt{\pi}}$

$$Ash(\kappa r); r < Ru(r) = Ash(\kappa R)exp(\kappa(R-r); r > R \tag{1}$$

Coefficient A defined by following condition: $\int_0^R u_1^2(r)dr + \int_R^\propto u_2^2(r)dr = 1$

here $u_1(r) = Ash(\kappa r)$ and $u_2(r) = sh(\kappa r)exp(\kappa(R-r)$.

Wave function and energy of excited P-state is:

$\psi_p(r) = \frac{v(r)}{r}\sqrt(\frac{3}{4\pi})cos(\theta)$

$$\frac{-1}{2}\frac{d^2v(r)}{dr} + \frac{1}{r^2}v(r) - V_0\delta(r-R)v(r) = -\frac{\kappa_1^2}{2}v(r) \tag{2}$$

where $\frac{\kappa_1^2}{2} = |E_p|$ -bound energy of p-state. replacing variable $\kappa_1 r = \rho$ lead to:

$$\frac{-1}{2}\frac{d^2v(\rho)}{d\rho^2} + \frac{1}{\rho^2}v(\rho) - \frac{V_0}{\kappa_1^2}\delta(\frac{\rho}{\kappa_1} - R)v(\rho) = -\frac{1}{2}v(\rho) \tag{3}$$

or it can be rewritten

$$\frac{-1}{2}\frac{d^2v(\rho)}{d\rho^2} + \frac{1}{\rho^2}v(\rho) - \frac{V_0}{\kappa_1}\delta(\rho - \kappa_1 R)v(\rho) = -\frac{1}{2}v(\rho) \tag{4}$$

replacing variable $v(\rho) = \sqrt(\rho)f(\rho)$ Equation (4) thus becomes

$$f''(\rho) + \frac{1}{\rho}f'(\rho) - [1 + \frac{(\frac{3}{2})^2}{\rho^2}]f(\rho) + \frac{2V_0}{\kappa_1}\delta(\rho - \kappa_1 R)f(\rho) = 0 \tag{5}$$

For areas where $\rho < \kappa_1 R$ and $\rho > \kappa_1 R$ this equations might be rewritten as

$$f''(\rho) + \frac{1}{\rho}f'(\rho) - [1 + \frac{(\frac{3}{2})^2}{\rho^2}]f(\rho) = 0 \tag{6}$$

i.e. Bessel equation with imaginary variable.

The solution at $\rho < \kappa_1 R$ at $\rho = 0$ is:

$$f(\rho) = AI_{3/2}(\rho) = A\sqrt{(\frac{2}{\pi\rho})}(ch\rho - \frac{sh\rho}{\rho}) = \frac{A'}{\sqrt{(\rho)}}(ch\rho - \frac{sh\rho}{\rho}) \tag{7}$$

and at the area of $\rho > \kappa_1 R$ it becomes:

$$f(\rho) = BK_{3/2}(\rho) = B\sqrt{(\frac{2}{\pi\rho})}exp(-\rho)(1 + \frac{1}{\rho}) = \frac{B'}{\sqrt{(\rho)}}exp(-\rho)(1 + \frac{1}{\rho}) \tag{8}$$

shsiv condition of comntinium function is

$$A'(ch(\kappa_1 R) - \frac{sh(\kappa_1 R)}{\kappa_1 R})) = B'exp(-\kappa_1 R)(1 + \frac{1}{\kappa_1 R}) \tag{9}$$

For sshivke derivatives we will take $v(\rho) = \sqrt(\rho) f(\rho)$

$$A'(ch\rho - \frac{sh\rho}{\rho}); \rho < \kappa_1 R v(\rho) = B' exp(-\rho)(1 + \frac{1}{\rho}); \rho > \kappa_1 R \tag{10}$$

$$\int_{\kappa_1 R - \epsilon}^{\kappa_1 R + \epsilon} d\rho [\frac{d^2 v}{d\rho^2} - \frac{2}{\rho^2} v(\rho) - v(\rho) + \frac{2V_0}{\kappa_1} \delta(\rho - \kappa_1 R) v(\rho)] = 0 \tag{11}$$

That can be solved very simply:

$$\frac{dv}{d\rho}|_{\kappa_1 R + \epsilon} - \frac{dv}{d\rho}|_{\kappa_1 R - \epsilon} + \frac{2V_0}{\kappa_1} v(\kappa_1 R) = 0 \tag{12}$$

Deviding (*) on (**) we get transcendent equation for κ_1.
Constant B' can be defined from condititon:

$$\int_0^R u_1^2(r) dr + \int_R^{\propto} u_2^2(r) dr = 1 \tag{13}$$

We can now to determine dipole moment of fullerene:

$$d = \frac{E}{\sqrt{3}} \int_0^{\propto} u(r) \cdot v(r) r dr \tag{14}$$

where $u(r)$ is the wave function of s -state and $v(r)i$ is the p-state. Then we can calculate α -polarisation of the fullerene molecules.

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