Screening Effect on Electric Field Produced by Spontaneous Polarization in ZnO Quantum Dot in Electrolyte

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INTRODUCTION

Voltage-gated ion channels are instrumental in living cells, as they play key roles in processes such as neuronal communication and muscle movement. At any given time, a cell has a specific membrane potential due to the separation of intracellular and extracellular ions such as K^+, Na^+, Ca^{2+} and Cl^-. When the membrane potential reaches a certain threshold, voltage-gated ion channels open, resulting in the flow of ions across the membrane. Theoretical and experimental studies have suggested that semiconductor nanoparticles with built-in spontaneous polarizations that are in close proximity to these ions channels can generate sufficient electric fields to affect the channels' dynamics [1-3]. This work calculates the strength of the electric field produced by ZnO quantum dots in physiological electrolyte.

THEORY

Considering a wurtzite quantum dot such as ZnO with its spontaneous polarization grown along the c-axis [4]. For such a quantum dot, it is possible to approximate the ZnO quantum dot as a uniformly polarized sphere as shown in Figure 1. Then the surface charge σ is given by

$$\sigma=\mathrm{P}\cdot\hat{n}=P\cos(\Theta) \tag{1}$$

By solving Gauss's law, the electric field produced from a ZnO quantum dot is

$$\mathrm{E}_{\mathrm{QD}}^{\mathrm{spon}}=\frac{P}{3\varepsilon}\frac{R^3}{r^3}\left[2\cos(\Theta)\hat{r}+\sin(\Theta)\hat{\Theta}\right],(r>R) \tag{2}$$

where ε is the dielectric function of the surrounding media. However in water-based electrolyte, the electric field produced from ZnO quantum dots decay exponentially due to the screening:

$$\mathrm{E}_{\mathrm{QD}}^{\mathrm{electrolyte}}=\mathrm{E}_{\mathrm{QD}}^{\mathrm{spon}}\,e^{-(r-R)/\lambda_D},(r>R) \tag{3}$$

where r is the distance from the center of the quantum dot, and λ_D is the Debye length. λ_D in electrolyte can be computed by

$$\lambda_D=\sqrt{\frac{\varepsilon k_B T}{2N_A e^2 I}} \tag{4}$$

where k_B is Boltzmann constant, T is temperature, N_A is Avogadro's number, e is elementary charge, and I is ionic strength of the electrolyte, which is given by $I=\frac{1}{2}\sum_{i=1}^{n} c_i z_i^2$, where c_i is the molar concentration of the ith ion in the electrolyte and z_i is the charge of the ith ion.

DISCUSSION

We found that, in the electrolyte consisting of 4 mM K^+, 126 mM Na^+, 3 mM Ca^{2+}, 1 mM Mg^{2+} and 138 mM Cl^- the Debye length is 16.02 nm. The screening effect caused by the electrolyte is shown in Figure 2. Considering that the minimum potential difference needed to switch a voltage-gated ion channel is of the magnitude of 6 mV, which requires the electric field across the 7 nm bilipid membrane of about 0.86×10^6 V/m, a ZnO quantum dot should be within 8.27 nm of the cell.

This knowledge is potentially relevant for therapeutic applications to treat medical conditions related to voltage-gated ion channels.

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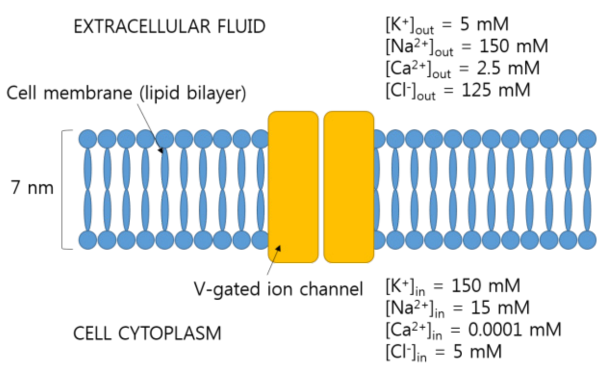

Fig. 1. Diagram of cell membrane with intracellular and extracellular concentrations of major ions.

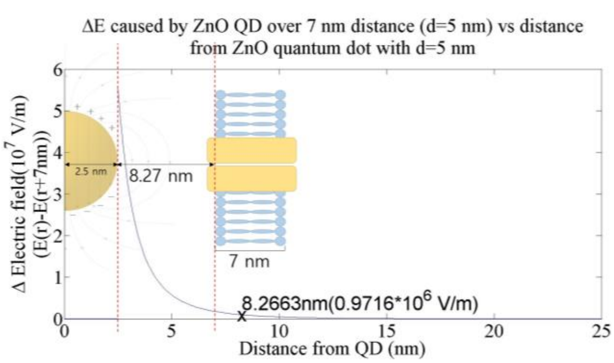

Fig. 2. Electric field produced from the spontaneous polarization of a ZnO quantum dot (diameter=5 nm) versus the distance from the quantum dot. The minimum distance required to switch an ion channel (8.27 nm) is indicated.

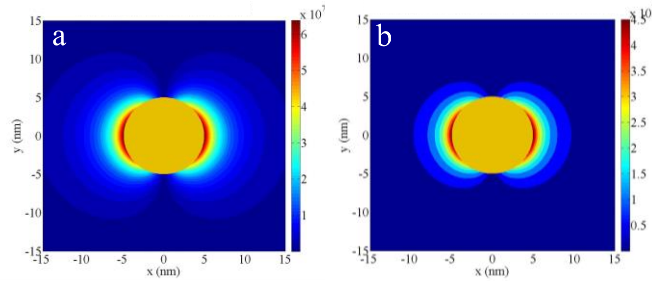

Fig. 3. Electric field due to spontaneous polarization of a 5-nm ZnO quantum dot in water (a) and in electrolyte (b).