Optical and Electrical Modeling of Three Dimensional Dye Sensitized Solar Cells

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Introduction: The goal of this work is to use a coupled optical and electrical COMSOL Multiphysics model to simulate dye sensitized solar cell (DSSC) based on photoanodes made of 3 dimensional (3D) indium tin oxide (ITO) nanorod architectures (Figure 1). The 3D photoanode is designed for improving the charge transport of the photo-generated electrons by providing the them closer conducting pathways near where they are formed to the contact to reduce the recombination loss.

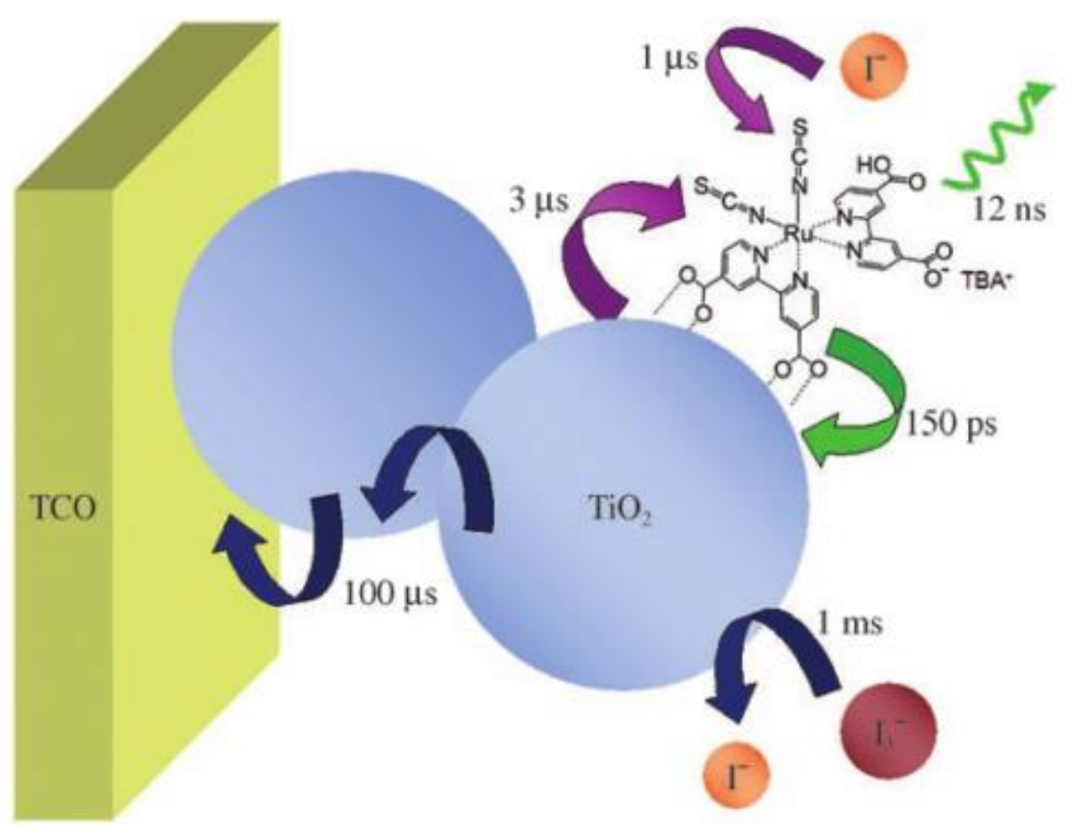
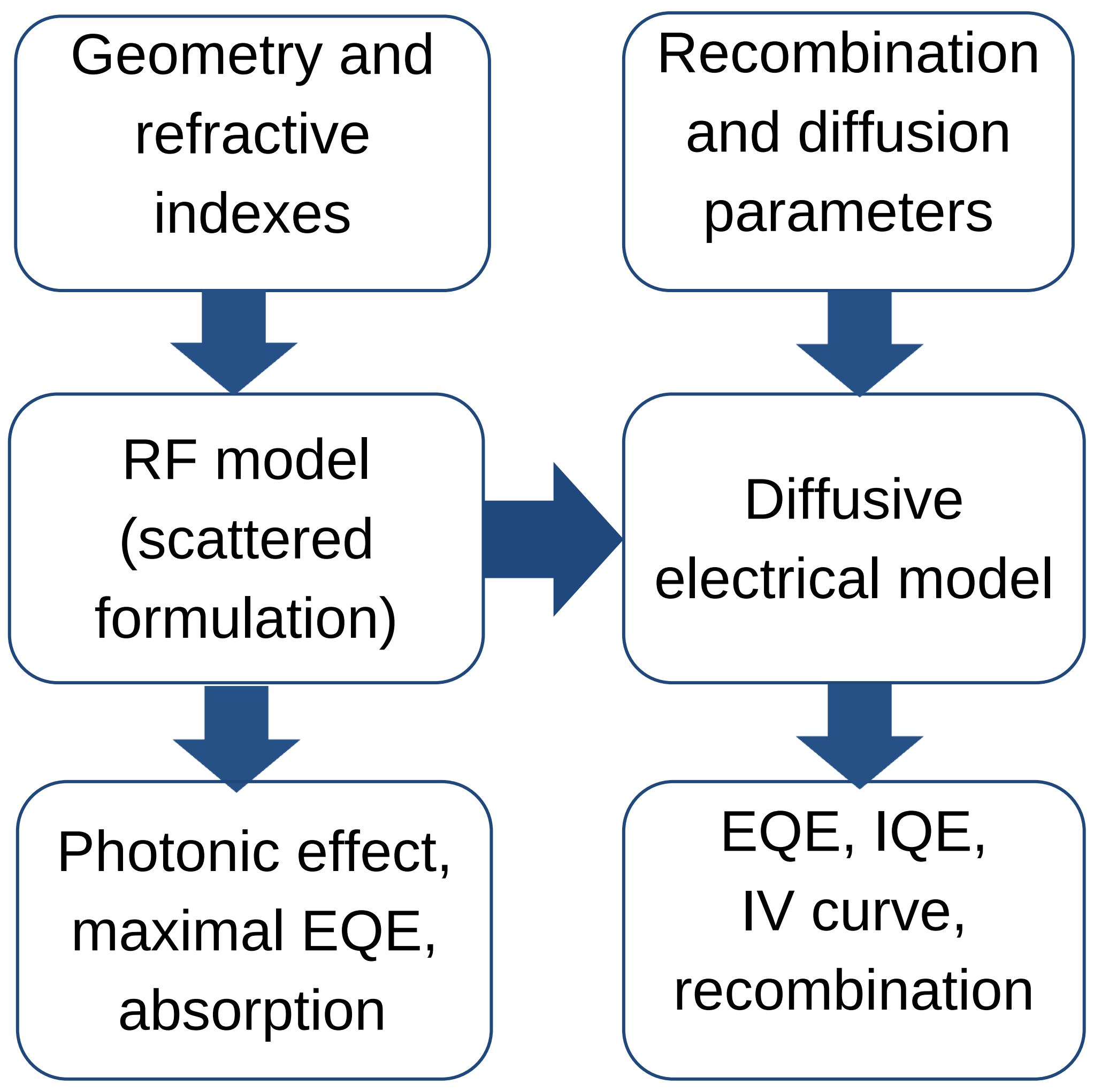


Figure 1. Kinetic processes of DSSC

Computational Methods: The model is a two-step optical-electrical coupled model as illustrated in Figure 2. In the first step, scattered field formulation enabled by RF module is applied to model the optical properties of the entire device stack. Coherence effect due to the substrate is considered by a generalized matrix method which is incorporated in the model. In the second step, 3D electron diffusion equation with the generation term obtained from the optical simulation is used to model the diffusion of the electrons within the TiO_2 network. Two assumptions are made for the electrical simulation. 1. High-ionic-strength electrolyte screens the electric field so there is no drift term. 2. Recombination rate of the electrons is linear with respect to the electron concentration in the TiO_2 conduction band.



Geometry and refractive indexes

Recombination and diffusion parameters

RF model (scattered formulation)

Diffusive electrical model

Photonic effect, maximal EQE, absorption

EQE, IQE, IV curve, recombination

Figure 2. Two-step coupled simulation design

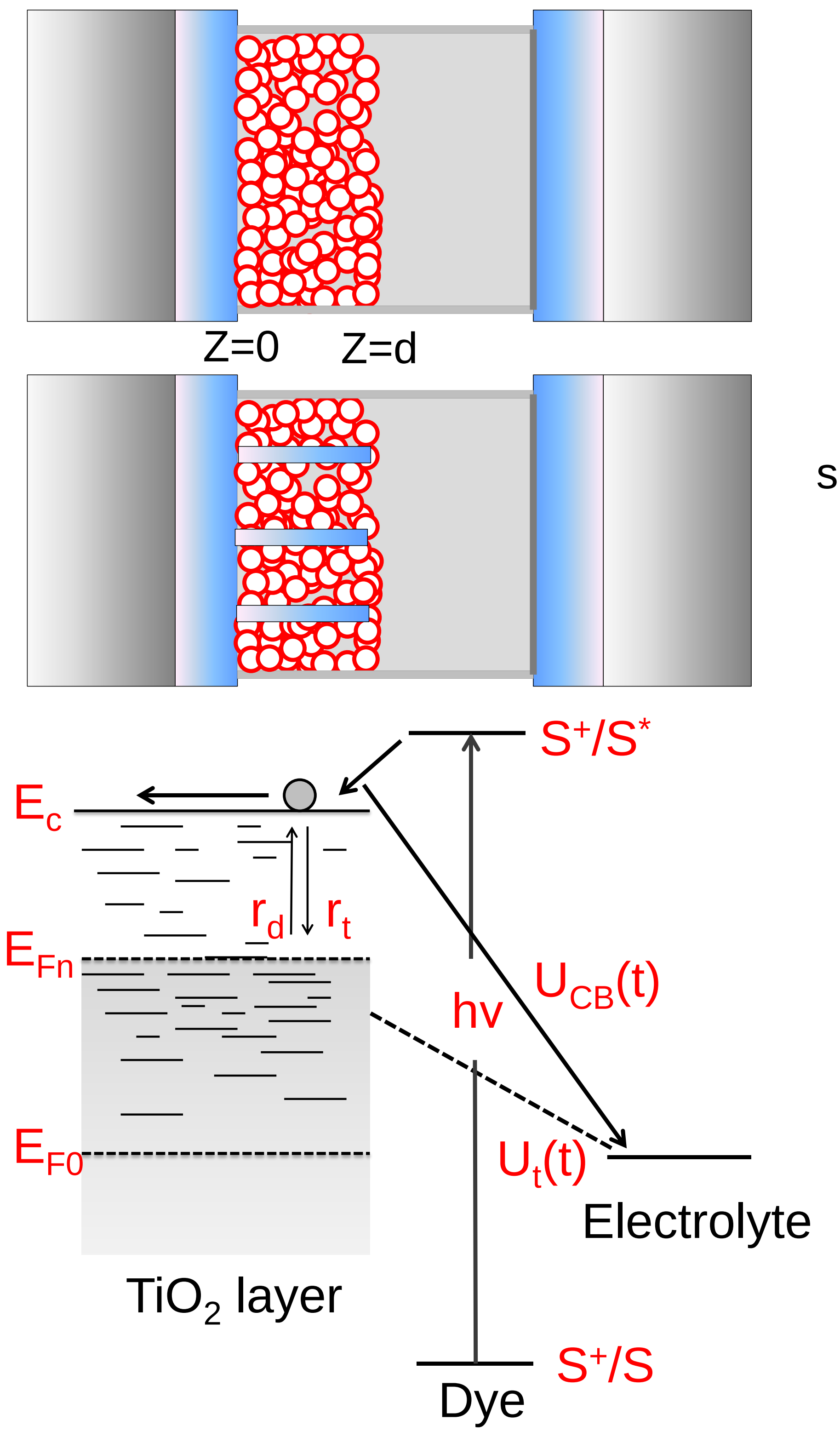


Figure 3. Illustration of the 2D and 3D DSSC structures, and the energy diagram

$$\begin{cases} \dfrac{\partial n_{cb}(\vec{r},t)}{\partial t} = \dfrac{1}{e}\dfrac{\partial \vec{j}(\vec{r},t)}{\partial \vec{r}} + G_e(\vec{r},t) - U_{cb}(\vec{r},t) - r_t + r_d \\ \dfrac{\partial n_t(\vec{r},t)}{\partial t} = r_t - r_d - U_t(\vec{r},t) \qquad n_{cb} = N_c f(E_c, E_{Fn}) \\ \vec{j}(\vec{r},t) = eD_0 \dfrac{\partial n_{cb}(\vec{r},t)}{\partial \vec{r}} \qquad U_{cb}(\vec{r},t) = (n_{cb}(\vec{r}) - \bar{n})/\tau_0 \end{cases}$$

$$\begin{cases} E_{F0} = E_{redox} \qquad V = \dfrac{1}{e}(E_{Fn}(0) - E_{F0}) \\ n_0\big|_{z=0} = N_c \exp\left[-\left(\dfrac{E_c - E_{Fn}(0)}{k_B T}\right)\right] \\ \dfrac{dn_{cb}}{dz}\bigg|_{z=d} = 0 \end{cases}$$

$$D_0 \nabla^2 n_{cb}(\vec{r}) - \frac{(n_{cb}(\vec{r}) - \bar{n})}{\tau_0} + G_e(\vec{r}) = 0$$

Figure 4. Equations for the diffusion model (left) and the boundary conditions (right)

Results: The external quantum efficiency (EQE) and the internal quantum efficiency (IQE) have been extracted from the simulation results. It is observed that the 3D architecture based electrode provides better photon to electron conversion efficiency especially at long wavelengths. This is due to a weak absorption coefficient of the dye molecule and the photo generated electrons are far from the electrode, where the 3D structure could make improvements.

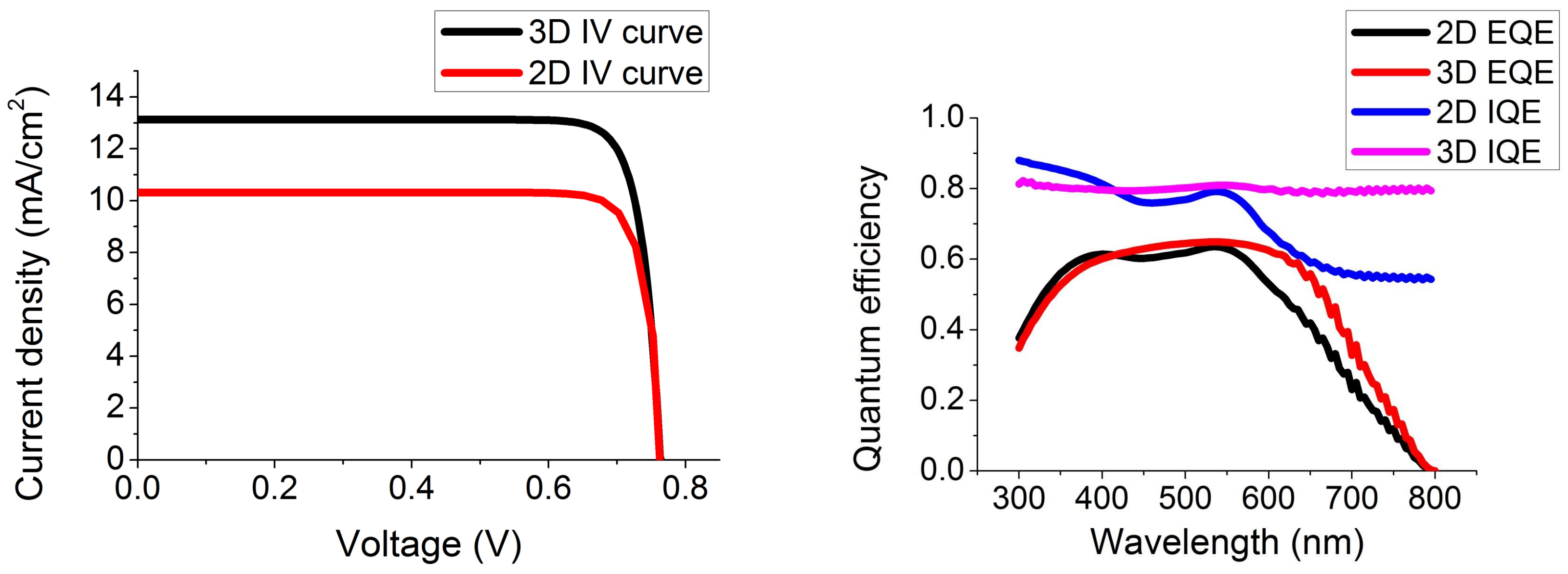


Figure 5. IV curve (left), EQE and IQE (right) of 2D and 3D based DSSC

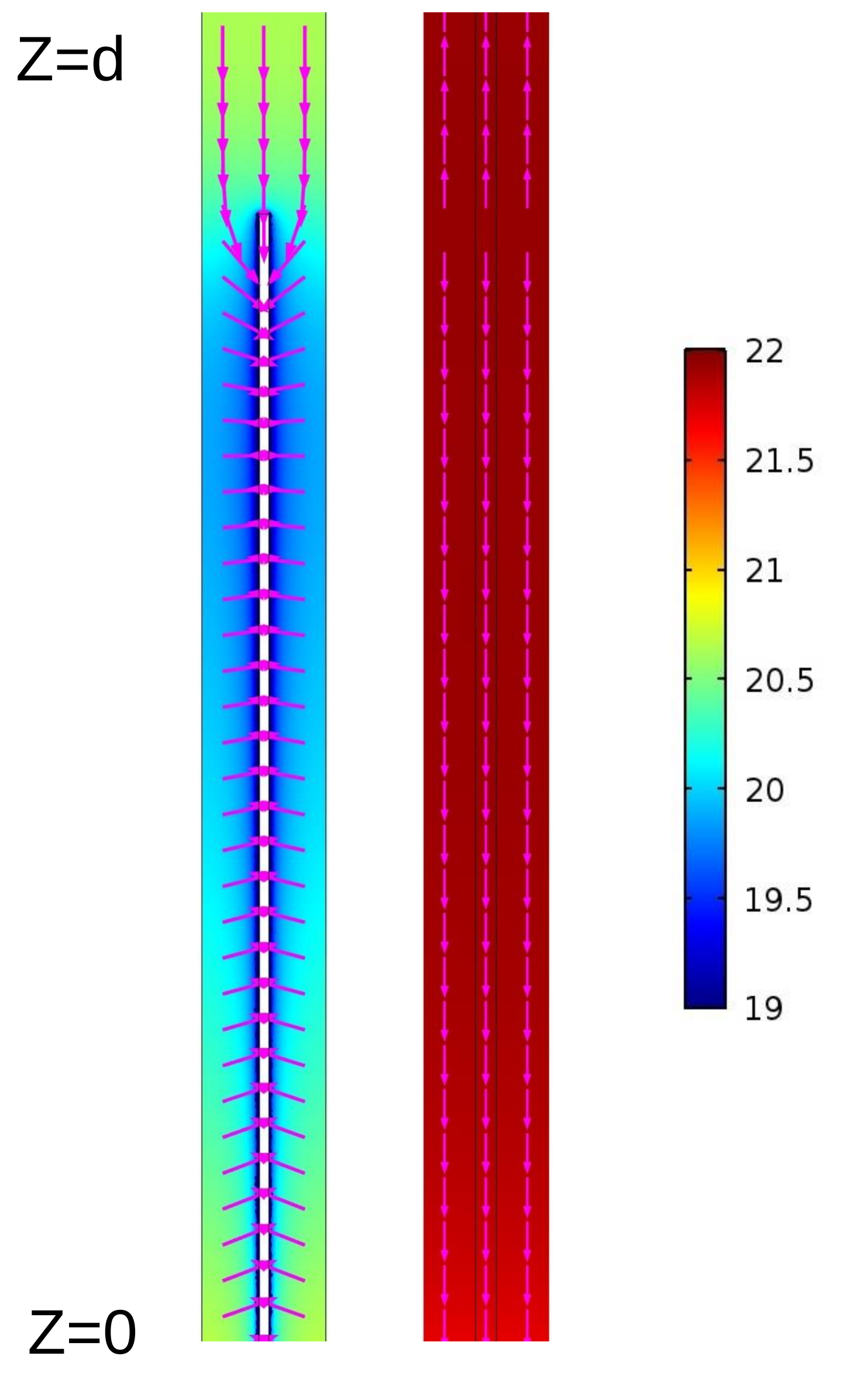


Figure 6. Electron concentration on $\log_{10}$ scale ($1/m^3$) and electron flow at short circuit

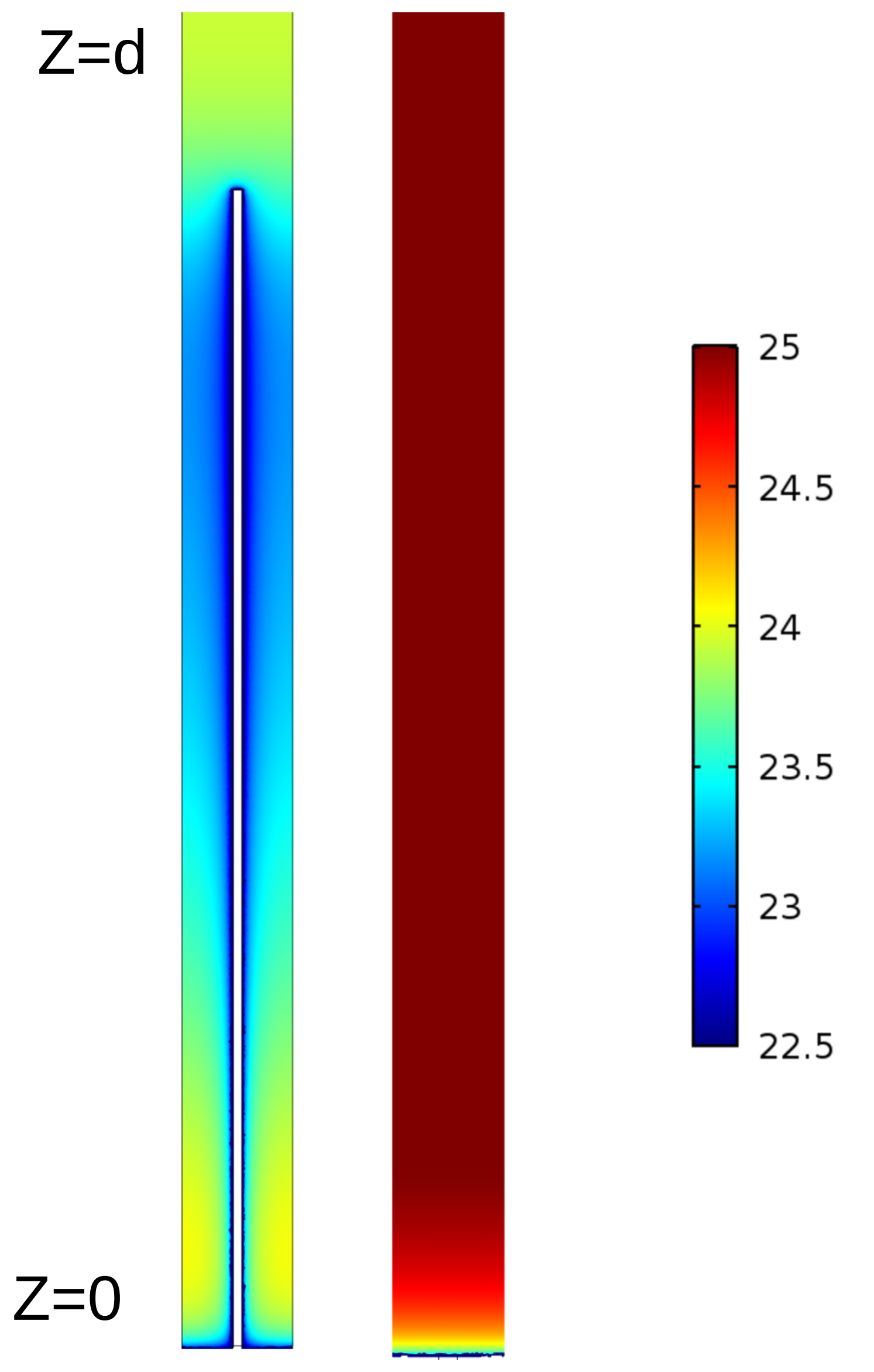


Figure 7. Recombination profile on $\log_{10}$ scale ($1/m^3/s$) at short circuit

Conclusions: We have used the two step optical –electrical coupled model to simulate DSSCs based on both planar (2D) and nanorod (3D) photoanodes. Useful information such as IV curve, EQE, IQE and recombination profile have been extracted to explain the advantages of the 3D electrode design comparing to the planar counterpart.

This model is now being used to simulate quantum dot sensitized solar cells. An electrical model based on both diffusion and drift current terms (with equations shown below) will be the future focus of the work to enable simulation of all solid state DSSC, and potentially organic solar cells with different morphologies.

References:

1. Byunghong Lee*, Peijun Guo*, Shi Qiang Li, D, Bruce Buchholz, R. P. H. Chang, 3D indium-tin-oxide nanorod array for charge collection in dye sensitized solar cells, in prep (* equal contribution)
2. L. M. Peter, Characterization and Modeling of Dye-Sensitized Solar Cells, The Journal of Physical Chemistry C, 111, 6601-6612 (2007)
3. Alex Martinson, Thomas Hamann, Michael Pellin, Joseph Hupp, New Architectures for Dye-Sensitized Solar Cells, Chemistry, 14, 4458-4467 (2008)
4. E. Centurioni, Generalized Matrix Method for Calculation of Internal Light Energy Flux in Mixed Coherent and Incoherent Multilayers, Applied Optics, 44, 7532-7539 (2005)
5. Sophie Wenger, Matthias Schmid, Guido Rothenberger, Adrian Gentsch, Michael Gratzel and Jurgen O. Schumacher, Coupled Optical and Electronic Modeling of Dye-Sensitized Solar Cells for Steady-State Parameter Extraction, The Journal of Physical Chemistry C, **115**, 10218-10229 (2011)
6. Guido Rothenberger, Pascal Comte and Michael Gratzel, A Contribution to the Optical Design of Dye-Sensitized Nanocrystalline Solar Cells, Solar Energy Materials & Solar Cells, **58**, 321-336 (1999)