Modeling and simulation Dye Solar Cells: extraction of parameters and trap states

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INTRODUCTION

The Dye Sensitized Solar Cell (DSC) is a very promising third generation photovoltaic device [1]. The light conversion mechanism is, however, quite different from any other solid state solar cell, resulting from the strong interplay between molecule excitation, electron transport and electrochemical processes involving ions. This complexity needs a reliable transport model able to catch the device as a whole and to describe experimental data. Moreover, DSCs are a prototype of electrochemical energy device and any model and simulation effort in this context can be easily transferred to other system such as fuel cells, batteries, water splitting devices etc.

In this communication we report on the work made to extend the multiscale simulator TiberCAD [2] to simulate DSC cell going beyond the simplifying assumption used so far. In fact, we treat trapped states, conductive charges, field profiles, and ion transport on equal footing. The developed model is also compared with experimental data and a sensitivity analysis is performed for the physical parameters entering in the model as a function geometrical/technological quantities such as the thickness of TiO2 layer or the type of electolyte .

MODEL AND DISCUSSION

The structure of the cell and the photo-conversion process are shown in fig. 1 and fig. 2, respectively .
Modeling DSC requires to handle four different charge carriers: e electrons, I_3^- and I^- ions and positive C cation necessary to assure the neutrality of the system.
For the charge transport we use a steady state drift diffusion equation for each carrier, coupled with the continuity and the Poisson equations [3]:

$$\begin{aligned} \nabla j_\gamma &= \Lambda_\gamma (G - R) \\ j_\gamma &= -D_\gamma \nabla n_\gamma + \mu_\gamma n_\gamma \nabla \varphi \\ \varepsilon \nabla^2 \varphi &= e(n_C + N_D^+ - n_{I_3^-} - n_{I^-} - (n_e - \overline{n}_e)) \end{aligned} \qquad (1)$$

The semiconducting structure is not perfectly crystalline therefore we need to consider an exponential distribution of trapped states that affect the mobility. The presence of the traps can be included in the model in an effective way (Multiple Trapping Model, [4]) modifying the expression of the diffusion coefficient [3] or considering real trapping states for electrons. A thorough investigation of the difference between the two models have been performed. We will show the influence of the traps on the determination of the electronic parameters comparing simulation results with experimental data (Fig.3).

It is generally accepted that the electronic current is diffusion driven because of the screening effect of the electrolyte[3] and many theories of transport in DSC are based on diffusion equation for electrons only[4]. However, we will point out the influence of the drift component of the current showing non negligible effects in presence of high density of trapped electrons (Fig. 4) or in particular DSC configurations.

CONCLUSION

A multiscale model is presented for DSCs. The parameterization of the model is obtain by comparison with experimental data and a sensitivity analysis is performed to assess the robustness of the funded parameterization. The influence of electron trapping states as well as the non negligible effects induced by the drift term is clearly pointed out. The obtained results are shielding new light on the description of the functioning of DSCs.

ACKNOWLEDGEMENT

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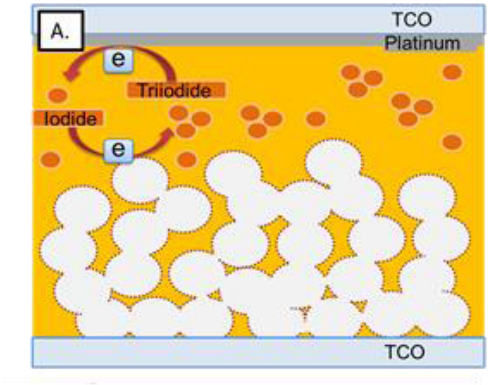

Fig. 1. Schematic representation of a DSC

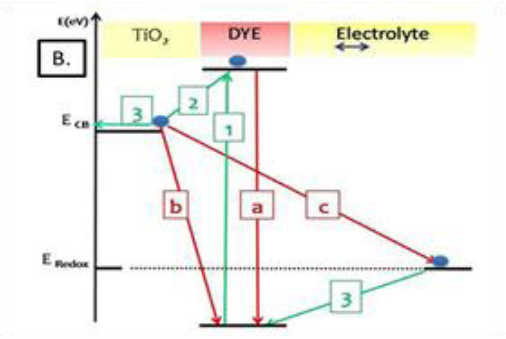

Fig. 2. Energy diagram of conversion processes: 1.Excitation of the dye, 2.Injection in the TiO_2, 3.Diffusion and collection at the anode. The recombination processes are: a. Decay of the dye in its ground state, b. Regeneration of the dye by TiO_2 conduction band electron, c. Reduction of the electrolyte occurring at the TiO_2 interface.

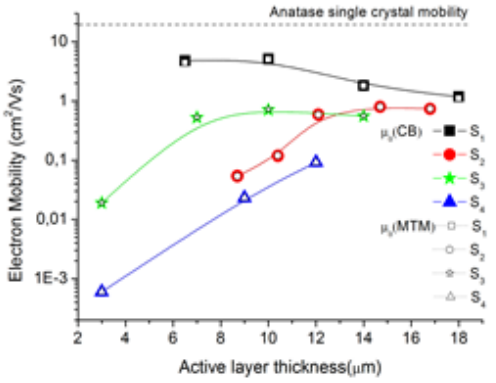

Fig. 3. Electron Mobility for different set of cells (colors) with increasing thickness. The calculation has been performed in Conduction Band Model and Multiple Trapping Model .

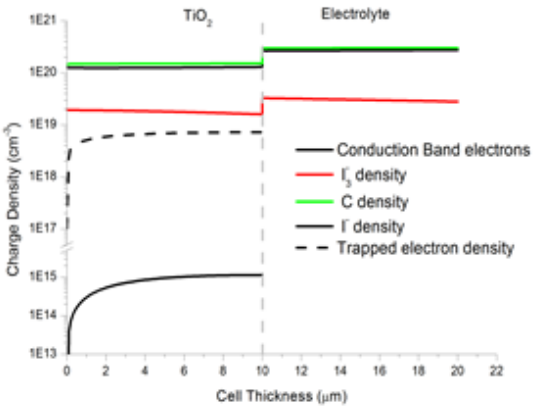

Fig. 4. Charge density profiles calculated for a typical cell with 10 μm active layer thickness. The conduction band (black continuous line) and the trapped(dashed black line) electron density are reported.