Optik - International Journal for Light and Electron Optics 169 (2018) 214–223

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.com/locate/ijleo

Original research article

Numerical simulation of highly efficient dye sensitized solar cell by replacing the liquid electrolyte with a semiconductor solid layer

Masood Mehrabian[a,*], Sina Dalir[b]

[a] Department of Physics, Faculty of Basic Science, University of Maragheh, P.O. Box 55136-553, Maragheh, Iran
[b] Department of Materials Engineering, Faculty of Engineering, University of Maragheh, P.O. Box 55136-553, Maragheh, Iran

ARTICLE INFO

Keywords:
Dye sensitized solar cell
Solid-state solar cell
Liquid electrolyte
Al-Modified titanium dioxide
P3HT

ABSTRACT

A dye-sensitized solar cell (DSSC) with FTO/TiO_2/Dye/Electrolyte/FTO structure was simulated by using SILVACO ATLAS software. To optimize the charge transfer at the TiO_2/dye/electrolyte interface, an Al-Modified TiO_2 layer was used and its influence on photovoltaic performance was investigated. Optimized solar cell showed maximum power conversion efficiency of 7.67% with short-circuit current of 16.50 mA/cm^2 and open-circuit voltage of 0.72 V at 100 mW cm^{-2} (1.5 A M).

To resolve the difficulties regarding the use of liquid electrolyte, a solid-state dye-sensitized solar cell (SS-DSSC) was simulated in which a P3HT layer acts as a hole collector instead of liquid electrolyte. SS-DSSC indicated a favorable performance deliver a short-circuit photocurrent of 12.70 mA cm^{-2} and open-circuit voltage of 0.67 V.

1. Introduction

Increasing worrying about the global warming due to consumption of fossil fuels has motivated researchers to look for renewable and non-polluting energy resources.

In this area, solar energy is abundant, clean and free energy resource which could be converted into electrical power in a pollution-free approach, called photovoltaic (PV) effect. Excitonic solar cells (XSCs) offer the hope of fabricating PV devices with high efficiency at low cost [1].

Excitonic solar cells include organic photovoltaics (OPVs), hybrid solar cells, Dye Sensitized Solar Cells (DSSCs) and Quantum Dot Sensitized Solar Cells (QDSSCs) belong to third-generation solar cells. Amongst all excitonic devices, DSSCs have an advantage of being flexible and ease of large-scale production than conventional silicon solar cells. DSSCs based on oxide semiconductors and organic dyes have recently emerged as promising approach to highly efficient solar-energy conversion.

To date, the most successful DSSC was fabricated based on TiO_2 thin film combined with a ruthenium based dye, as reported by Gra¨tzel's group in 1991 [2–4]. They successfully developed the first efficient DSSC with light power conversion efficiency > 7% which ensures an extensive field to study on DSSCs during the following years.

A dye-sensitized solar cell (DSSC) consists mainly of transparent conducting oxide (TCO) substrates, a semiconductor thin film electrode, monolayer of dyes adsorbed onto the surface of electrode, and solid or liquid electrolyte and platinum electrode [5].

In DSSCs absorption of photon happens due to presence of dye monolayer which further leads to creation of excitons (electron-hole pairs). These excitons must be dissociated for charge generation. The photo-electron is transferred into the conduction band of semiconductor available as photo anode and holes leaving the opposite side of device by means of a liquid electrolyte composed of a

* Corresponding author.
E-mail address: masood.mehrabian@maragheh.ac.ir (M. Mehrabian).

https://doi.org/10.1016/j.ijleo.2018.05.059
Received 26 March 2018; Accepted 16 May 2018

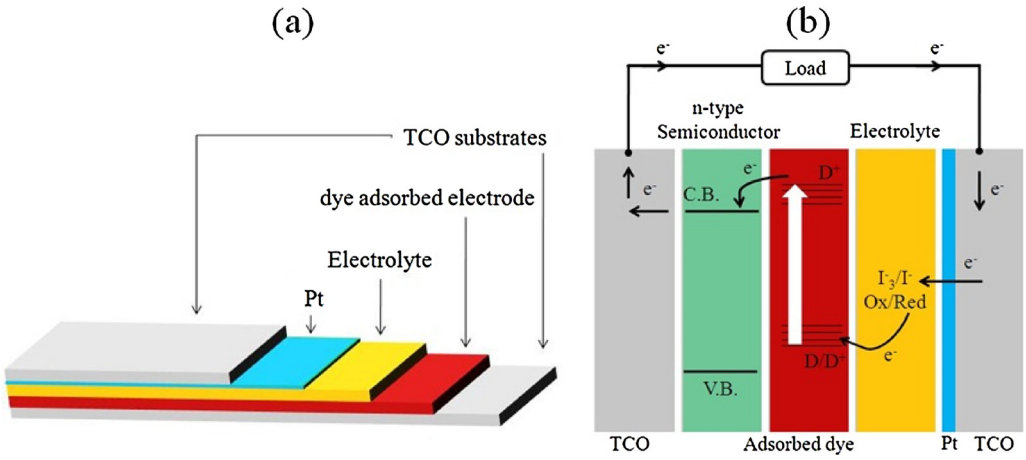

Fig. 1. (a) Schematic diagram of a dye sensitized solar cell (DSSC), (b) the working principles of DSSC.

redox couple (I_3^-/I^-) [6].

A schematic diagram as well as the working principle of a dye-sensitized solar cell is shown in Fig. 1.

In present study, a DSSC with FTO/TiO_2/Dye/Electrolyte/Pt doped FTO structure was simulated by using SILVACO ATLAS TCAD software. Then the TiO_2 layer was replaced with Al doped TiO_2 to optimize interfacial charge transfer process. Finally the performance characteristics of these cells were compared with the results reported in the literature [7].

1.1. Working principles of DSSCs

DSSCs are photo-electrochemical systems containing of:

(1) A transparent conducting oxide (TCO) glass substrate like fluorine-doped tin oxide (FTO),
(2) A porous oxide thin film, an n-type semiconductor, (i.e., TiO_2), with adsorbed dye molecules as the photo-anode,
(3) A platinized FTO glass (Pt:FTO) as the counter electrode, and
(4) A liquid electrolyte containing a redox couple as a conductor to electrically connect the two electrodes.

For highly efficient solar cells, the presence of a compact blocking layer between the FTO and the porous oxide thin film, has been shown to be essential [8].

The working principle of the dye-sensitized solar cell (DSSC) is presented in Fig. 1(b). During light illumination, Photons strike the cell and their energy is absorbed by dye molecules. Depending on the dye used, different energy levels of photons may be absorbed. The adsorbed photons generate excitons. D & D^+ signify the ground and excited states of the dye. C.B. and V.B. denote the energies of the lower edge of the conduction band and upper edge of the valence band of TiO_2, respectively. Inorganic/organic interfaces are formed between the TiO_2 particles and the dye molecules. To create electrical current, these generated excitons should be rapidly split at the surface of the oxide film. Electrons are injected to the conduction band of the TiO_2 film, leaving the dye in the oxidized state (D^+). These photo-electrons flow through the external load to the counter electrode where they reduce the redox species through following reaction:

$$I_2 + 2e^- \rightarrow 2I^- \quad (1)$$

Then, the reduced part of the couple regenerates the photo-oxidized dye. That is, the dye molecules are regenerated through following reaction:

$$D^+ + I^- \rightarrow D + {}^1\!/_2 I_2 \quad (2)$$

Thus, the light energy is converted to electrical energy without any net chemical reaction.

1.2. Solar cell modeling

The first step in modeling of a solar cell is specifying the mesh on which the device will be constructed and Schrödinger's equations will be solved.

ATLAS solves these one-dimensional (1D) equations along a series of slices in the y direction relative to the device.

To do this, the locations of individual mesh lines and their local spacing must be determined using the X.MESH L, Y.MESH L, X.MESH S and Y.MESH S statements, respectively.

The following 1D Schrödinger equation should be solved for eigen-state energies $E_n(x)$ and wave-functions $\Psi_n(x, y)$ at each slice perpendicular to x-axis and for each electron: