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The Chemistry and Physics of Dye-Sensitized Solar Cells

William A. Vallejo L., Cesar A. Quiñones S. and Johann A. Hernandez S.
Universidad Nacional de Colombia,
Universidad de Cartagena
Universidad Distrital F.J.D.C, Bogotá,
Colombia

1. Introduction

Climate change is one of the major environmental problems that affect our society. At present annually more than 40 billions Tons of greenhouses gases are exhausted to atmosphere and the tendency is to the rise; the main reason for this situation is the high and uncontrolled use of fossil resource in energy generation. Development an environmental, friendly and reliable energy technology is a necessity. Solar Energy emerged as possible solution to confront this problem. This technology permits a direct conversion of sunlight into electrical power without exhaust of both greenhouse gases and another polluting agent. Actually silicon technology is market leader in photovoltaic technologies, however since a pioneering (Grätzel & O’Regan, 1991) dye-sensitized solar cells (DSSCs) have become in one important and promising technology in photovoltaic field. DSSCs given born to new solar cells generation replaced classical solid-state homo and hetero-junction device by a new concept with a nano-working electrode in photo-electrochemical cell. This technology offers a very low cost fabrication and easy industry introduction prospective; furthermore efficiencies near to 10% AM1.5 for DSSCs have been confirmed. DSSCs consists of three main components: A dye-covered nanoporous TiO$_2$ layer on a glass substrate coated with a transparent conductive oxide (TCO) layer, an redox electrolyte and a electrical contact deposited on conducting glass. Different parameters affect efficiency of the DSSCs: types of materials used as electrolyte, dye and electric contact, and synthesis method used to obtain these materials. In this chapter DSSCs components and different aspects related with photovoltaic principles and DSSCs performance will be studied. Special emphasis will put on to review physical, chemical and electrochemical principles of DSSCs operation.

2. Mechanism operation

All photovoltaic devices present two important steps to convert sunlight into electrical energy:
1. Radiation absorption with electrical excitation.
2. Charge carriers separation.

The way which radiation is absorbed and carriers are separated are two of the main differences between DSSCs and classical p-n junction. Conventional photovoltaic principle
relies on differences in work functions between the electrodes of the cell in which photogenerated carriers could be separated, an asymmetry through cell is necessary to obtain electrical power. In classical p-n junction of solid state device the separation of photogenerated carriers relies on separation through depletion region built at p-n interface materials (Neamen, 1997). A different process occurs in DSSCs. Figure 1 shows typical scheme for DSSCs. The working electrode of DSSCs is conventionally constituted by mesoporous network of TiO$_2$ nanocrystalline (5-15µm, thickness) covered with a dye monolayer (conventionally Ru complex); this working electrode is supported on conducting glass (transparent conducting oxide, TCO). Different materials as platinum, palladium and gold could be use as counter-electrode of the cell; finally the gap between the electrodes is typically filled with a molten salt which containing a redox couple (A/A$^-$); this salt is a hole conductor. Most DSSCs studied so far employ redox couple as iodide/tri-iodide (I$^-$/I$_3^-$) couple as electrolyte because of its good stability and reversibility (Pooman & Mehra), however others hole conductors as solid and ionic electrolytes also can be used. In overall process, the DSSCs generate electric power from light without suffering any permanent chemical transformation (Kelly & Meyer, 2001)

Fig. 1. General Structure of a dye-sensitized solar cell, the electron migration is showing.

In DSSCs, the basic photovoltaic principle relies on the visible photo-excitation of dye molecule; the esquematic reaction of overall process is follows:

$$\text{TiO}_2/D + h\nu \leftrightarrow \text{TiO}_2/D^{*}_{\text{LUMO}}$$  \hspace{2cm} (1)

$$D^{*}_{\text{LUMO}} + CB_{\text{TiO}_2} \rightarrow \text{TiO}_2/D^{*} + e_{CB}^-$$  \hspace{2cm} (2)

$$\text{Pt} + [I_3^-] \rightarrow 3I^-$$  \hspace{2cm} (3)

$$\text{TiO}_2/D^{*} + 3I^- \rightarrow [I_3^-] + D$$  \hspace{2cm} (4)

$$e_{CB}^- + D_{\text{HOMO}} \rightarrow D + CB_{\text{TiO}_2}$$  \hspace{2cm} (5)

$$e_{CB}^- + [I_3^-] \rightarrow 3I^- + CB_{\text{TiO}_2}$$  \hspace{2cm} (6)
Fig. 4. Unit cell for: (a) anatase TiO\textsubscript{2} and (b) rutile TiO\textsubscript{2}.

Fig. 5. XRD pattern of TiO\textsubscript{2} thin film, (take it on Shimadzu 6000 diffractometer with Cu-K\textsubscript{\alpha} radiation (\(\lambda = 0.15418\) nm) source.

<table>
<thead>
<tr>
<th>Crystal Structure</th>
<th>System</th>
<th>Space Group</th>
<th>Lattice constant (nm) A</th>
<th>B</th>
<th>c</th>
<th>c/a</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rutile</td>
<td>Tetragonal</td>
<td>(D_{4h}^{14} - P4_{2} / mnm)</td>
<td>0.4584</td>
<td>--</td>
<td>0.2953</td>
<td>0.644</td>
</tr>
<tr>
<td>Anatase</td>
<td>Tetragonal</td>
<td>(D_{4h}^{14} - I4_{1} / amd)</td>
<td>0.3733</td>
<td>--</td>
<td>0.937</td>
<td>2.51</td>
</tr>
<tr>
<td>Brookite</td>
<td>Rhombohedral</td>
<td>(D_{3h}^{15} - P6\bar{3}c)</td>
<td>0.5436</td>
<td>0.9166</td>
<td>0.5135</td>
<td>0.944</td>
</tr>
</tbody>
</table>

Table 1. TiO\textsubscript{2} bulk properties
With respect to metal polypyridine complexes, organic dyes have been less investigated for sensitization of wide band gap semiconductors. Apart from the coumarin derivative, organic dyes such as porphyrins, phthalocyanines, perylene bis-amides, xanthenes and polyenes show low photon to electron conversion efficiencies. The understanding of the factors that determine these low performances could lead to the development of new efficient dyes, cheaper to manufacture than transition metal complexes (Argazzi et al, 2004). Figure 8 (a) shows some typical molecular structure of a basic phthalocyanine, (special polypyridine complexes); in this figure, $R$ means a radical like: $t$-butyl, $n$-hexyl, $n$-octyl, in some cases $R$ can be a substituted amine, and $M$ means a metallic cation. Figure 8(b) shows some organic dye sensitizers used in DSSCs; TA-St-CA nad TA-TM-TA dyes contain a $p$-conjugated oligo-phenylenevinylene unit with an electron donor-acceptor moiety for intramolecular charge transfer, and a carboxyl group as an anchoring unit for the attachment of the dye onto TiO$_2$ nanoparticles; efficiencies about 9% have been reported for DSSCs based in organic dyes. Additionally, C217 dye employing a lipophilic dihexyl oxy-substituted triphenylamine electron donor, a cyanoacrylic electron acceptor, a distinguishable feature of this new amphiphilic D–π–A chromophore consists in a binary $n$-conjugated spacer. Here, an electron-rich 3,4-ethylenedioxythiophene unit is connected to electron-donor to lift the energy of the highest occupied molecular orbital (HOMO), while thienothiophene conjugated with A leads to a suitable lowest unoccupied molecular orbital (LUMO) energy; DSSCs based on C217 dye have reported efficiencies about 9.8%.