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Effect of DNA-TiO_2 Scaffold as Sensitize Absorber in Dye Sensitized Solar Cell

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ABSTRACT

To lower cost per watt demand, Photo-electrochemical (PEC) cell based Dye Sensitized Solar cell (DSSC) becomes one of promising alternative than currently market leading crystalline-silicon-based photovoltaic solar cell. DSSC fabrication cost is very low as it uses abundant and non toxic and non scarce materials and also has some properties like flexibility, semitransparent and aesthetic etc. DNA is very low cost nano-dimensional material with excellent nano-template and electrical properties. Also DNA has two most unique properties are its double strand recognition and a special structuring due to self assembly which improves optical utilization due to its symmetrical double-helix structure. The DSSC has low efficiency than crystalline silicon solar cell, so further improvement in DNA based DSSC efficiency and lifetime which further reduces cost/watt. Then it can be extensively used in various applications.

General Terms

Absorption, Double stand, Backbone, Photo-electrochemical, Exciton, Efficiency, Intensity, base pair, Quantum efficiency, Spectrum, Incident photon, Hole transporters, Concentration gradient, Electrolyte, Sensitizer

Keywords

DNA, Dye sensitized solar cell, Double helix, DNA tiling, DNA origami, DNA-CTMA, BSF

1. INTRODUCTION

Due to ever increasing global energy demands, all natural non renewable energy sources like fossil fuels are firstly depleting and causes of environment and ecological damages. So, recent trends in energy supply are going for to use renewable energy. Among of them solar energy is most promising as it is more steady, reliable and easily available at zero cost. Another advantage is the solar energy incident on the earth surface is about 1650 TW/sec is much higher than the combined power consumption by our world is about 20TW using traditional energy sources. Thus the solar energy has pre-advantages to produce more electricity. For this purpose, a demand for large scale production of solar cell has been emerged commercially.

Solar cell is device that converts solar energy into electricity by the photovoltaic effect. From the beginning to still now, there are several proposals for solar cell design on the basis of used materials, techniques and photovoltaic conversion efficiency(η) etc. Market leading photovoltaic solar cell is basically first generation solar cell of which crystalline silicon solar cell is most popular with efficiency 12%-16% depending on manufacturing procedure and wafer quality. Silicon are abundantly available in nature, get in purest form, also have excellent electrical properties with bandgap 1.1ev.But first generation solar cell has several disadvantages-high material cost, high processing cost The second generation solar cells are based on thin film technology with wet process at low temperature that lowers cost/watt. The materials are amorphous silicon (a-Si), cadmium indium selenide (CIS), indium tin oxide (t-Si). Another advantage is the use of flexible substrates which leads more part in the energy conversion sector. But these solar cells also have several drawbacks as conversion efficiency is not so high, toxic and scarce materials are used. According to Schockly and Queisser limit, the first and second generation solar cell can achieve the maximum efficiency upto 31% and the third generation solar cells are based on newest techniques with more abundant and non-toxic materials can achieve the conversion efficiency more than Schockly-Queisser limit thus lowers cost/watt. The Dye sensitized solar cells (DSSC) are belongs to this group given in [1]. It is basically photoelectrochemical(PEC) operation based on exciton-diffusion of charge carriers.

DNA stands for deoxyribonucleic acid, carries the genetic information. DNA and electronics seem to be two different things, but a series of events has highlighted the unusual ability of DNA to form electronic components. Two of the most unique properties of DNA for molecular electronics are its double strand recognition and a special structuring due to self assembly as in [2].

2. WHAT IS DNA?

DNA, deoxyribonucleic acid, encodes the architecture and function of cells in all living organisms.

2.1 DNA Structure

DNA, shown in Figure 1, is made of a sequence of four bases: thymine (T), cytosine (C), adenine (A), guanine(G), attached to phosphate-sugar backbone as in [3].Two strands may come together through hydrogen bonding of the bases A with T(AT) and G with C (GC). In 1953, the 3D model of double helix structure has been discovered by Watson and Crick.

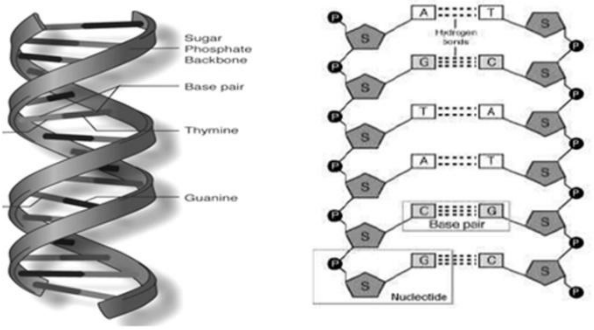

Fig 1: DNA double helix with ladder diagram.

The DNA double helix is made of two strands, which are each a sequence of four bases attached to a Phosphate-Sugar backbone. The bases opposite each other on the two strands are bonded by hydrogen bonds. (b) Schematic of the chemical structure of the Phosphate-Sugar backbone of a single strand of DNA.

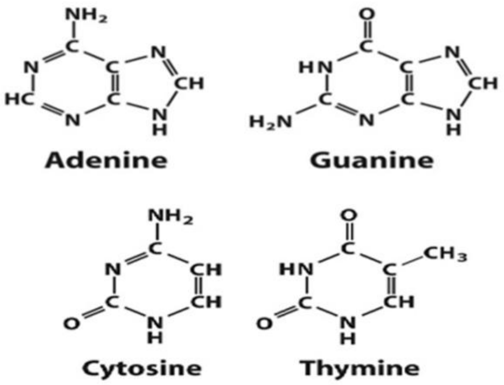

Fig 2: The four bases that compose DNA: (a) Adenine, (b) Guanine, (c) Cytosine., and (d) Thymine.

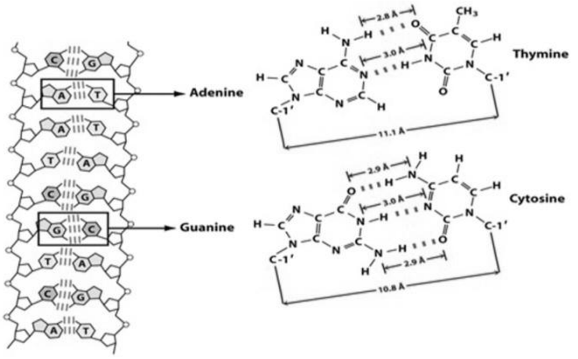

Fig 3: Base pair sequence (A-T and G-C) of DNA.

DNA is a macromolecule made of four different monomers. Each monomer unit, called a nucleotide, consists of a phosphate group, a 2-deoxyribose (a 5-carbon sugar), and one of four bases shown in Figure 2. Double-stranded DNA is due to hydrogen bonding between bases on two single strands. In this case, the bases come together is called Watson–Crick base pair. The A base only pairs with T, and the G base only pairs with C. These pairs allow for the formation of the double helix, a secondary structure of DNA. The carbons which bond to the phosphate-sugar backbone on each side of either base pair are the same distance apart, which allows for the regular structure of the helix.

To understand what the double helix of DNA itself looks like (Figure1), imagine it as a long, straight ladder with flexible uprights and ten solid, flat, horizontal rungs. Facing the ladder, keep the base still, and take the top of each upright in one hand. Then twist the uprights around, pushing the right upright away from you, and pulling the left upright towards you. Carry on twisting until the tops of the uprights are back to where they started, having travelled through 360 degrees. The rungs remain parallel to the ground. Now you have a rather large outline model of one complete turn of the DNA double helix (one helix from each upright) with ten base pairs. DNA goes on for many thousands of base pairs in this way. They consist of a regular arrangement of a type of sugar, called deoxyribose, with small chemical Phosphate groups.

In a straight ladder, the supporting uprights have to be kept the same distance apart. In DNA, the uprights are the same distance apart because each rung is made from a pair of particular chemicals called bases. One base of each pair is a purine (the purines which go into DNA are guanine and adenine); the other base of each pair is a pyrimidine (the pyrimidines which go into DNA are thymine and cytosine). The purines are bigger than the pyrimidines, but the two purines are about the same size as each other, and the two pyrimidines are also about the same size as each other. Since all the ‘rungs’ or base pairs have to contain one purine and one pyrimidine, they will all be about the same size.

2.2 DNA selfassembly

From this previous section, Adenine (A) is hybridized with Thymine (T) only through two weak hydrogen bonds and Guanine (G) is bonded with Cytosine(C) only through three weak hydrogen bonds. There are several models for DNA assembly – single stand, double stand, triplet and cross tile etc.DNA tiling is based on cross tiling with junctions and sticky-ends which are exploited for this purpose. Sticky end is some unoccupied bases in a single stand which are further larger than other in cross tile and often used to combine two DNA nanostructures together via hybridization of their complementary base. A typical DNA cross tile with junction and sticky end is shown below.

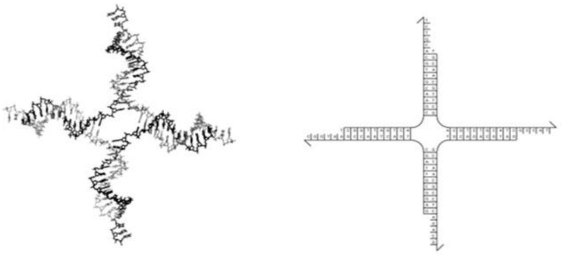

Fig 4: DNA cross tiling with junction and sticky end.

DNA tile is a DNA nanostructure that has a number of sticky ends on its sides. A DNA lattice is a DNA nanostructure composed of a group of DNA tiles that are assembled together via hybridization. A typical DNA lattice using number of DNA tiles is shown in figure below.

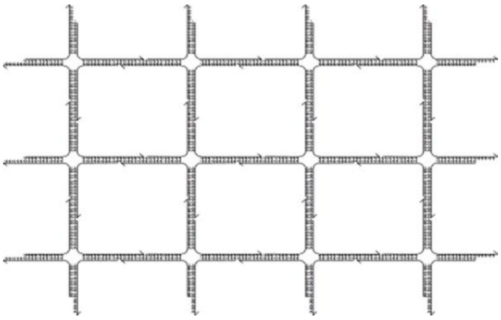

Fig 5: DNA lattice with number of DNA tiles.

DNA Origami, another way of newest self-assemble of two dimensional nanoscale patterns. In this technique, the double helix structure is rasterized make pattern for along single stand scaffold nucleotide sequence and a pattern for short staple strands. Then these are synthesized and mixed in solution and self-assemble into the target two dimensional shapes as shown in figure below.

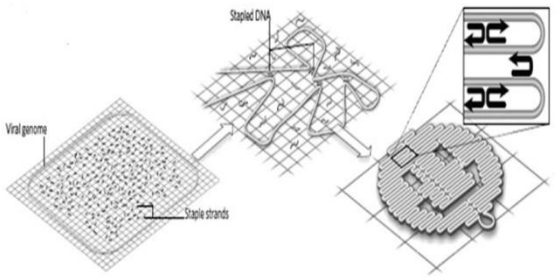

Fig 6: DNA Origami based self assembly.

3. PHOTOVOLTAIC SOLAR CELL

Photovoltaic solar cell converts photon energy into electrical energy as similar operation as pn junction diode. According to concentration gradient, the majority carriers are diffused in each other and minority carriers are recombined at the barrier of the junction as in [4]. If the energy of the incident photon has greater than or equal to the band gap energy, then electron (e)-hole(h) pair components will be generated. The basic solar cell and it's equivalent circuit diagram is shown in figure 4.

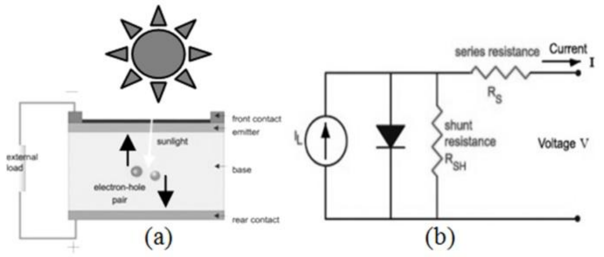

Fig 7: Basic Solar cell structure with equivalent circuit diagram.

From this circuit, there are some circuit components like light current (I_L), series resistance (R_S), shunt resistance (R_{SH}) which are inherent properties of solar cell.

3.1 Solar cell characteristic

The generated photocurrent in a solar cell under illumination is dependent on the incident light wavelength and intensity. This circuit current can be expressed by.

$$I_L = q \int_E^{E+dE} bs(E)QE(E)\,dE \tag{1}$$

where *QE(E)* is the quantum efficiency, the probability that an incident photon of energy E will deliver one electron to external circuit and *bs*(*E*) is the incident spectral photon flux density. The number of photons of energy in the range *E* to *E+dE* which are incident on unit area in unit time and *q* is the electronic charge. Quantum efficiency is dependent on the absorption coefficient of the material, the efficiency of charge separation and collection. The dark current density I_{dark} is defined as

$$I_{dark} = I_0\left[\exp\left(\frac{qV}{nkT}\right) - 1\right] \tag{2}$$

The overall current of a solar cell under illumination can be approximated as the sum of light current and dark current, which can be expressed as Eq. (3)

$$I = I_L - I_0\left[\exp\left(\frac{qV}{nkT}\right) - 1\right] \tag{3}$$

When the cell is short circuit i.e. $v=0$, then short-circuit current becomes $I_{SC} = I_L$ and when the cell is isolated, the potential difference will reach its maximum, the open circuit voltage, under a certain level of illumination.

$$V_{OC} = \frac{nkT}{q}\ln\left(\frac{I_L}{I_0} + 1\right) \tag{4}$$

The solar cell delivers power in the bias range from 0 to *Voc*. The output power of a cell reaches its maximum at the optimum operating point. This occurs at some voltage V_{MP} with a corresponding current I_{MP} as shown in figure 5.

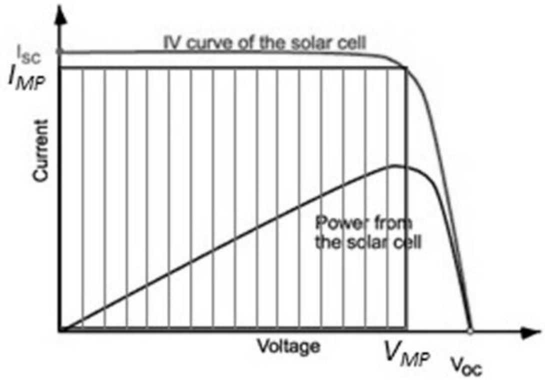

Fig 8: Solar cell VI characteristic.

The fill factor is defined as the ratio of maximum power to the product of open circuit voltage and short circuit current. It is a measure of the "squareness" of the IV curve.

$$FF = \frac{V_{MP}I_{MP}}{V_{OC}I_{SC}} \tag{5}$$

The efficiency of a solar cell is determined as the fraction of incident power P_{in} which is converted to electricity.

$$\eta = \frac{V_{OC}I_{SC}FF}{P_{in}} \tag{6}$$

All the above mentioned four quantities, *Voc*, *Isc*, *FF*, η are essential parameters for solar cell characterization.

4. DYE SENSITIZED SOLAR CELL

The conventional dye sensitized solar cell (DSSC) has been first proposed by Grätzel. Thus it is also named as Grätzel cell, based on a semiconductor formed between a photo-sensitized anode and an electrolyte, a photo electrochemical (PEC) material. A typical diagram of dye sensitized solar cell is shown below.

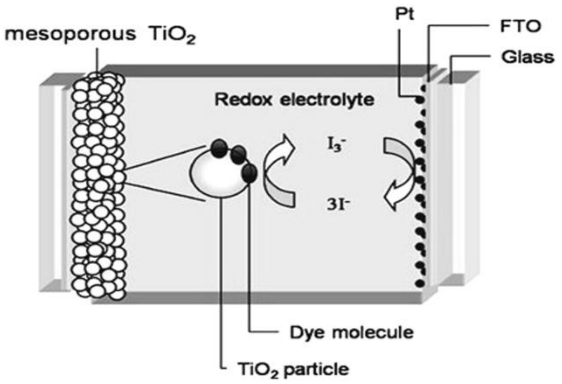

Fig 9: DSSC structure with energy band.

The mechanism of DSSC is as sunlight enters the cell through the transparent cover, striking the dye on the surface of the TiO2. This creates an excited state of the Ruthenium based dye, from which an electron is injected into the conduction band of the TiO2. Electrons then flow out of the TiO2 from the anode. The dye molecule loses an electron and so the oxidized dye needs to be regenerated, and hence an electrolyte / hole transport layer is necessary as in [6]. Traditionally, an I-/I3- liquid redox electrolyte has been used for this purpose. The charge transfer mechanism and energy band of DSSC is shown below.

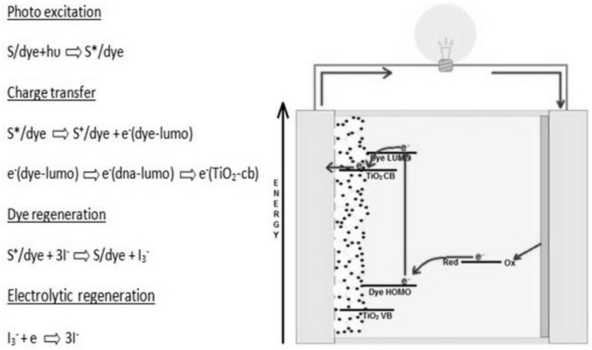

Fig 10: Charge transfer mechanism with energy band.

For selection of Ruthenium based dye, the flow DSSCs are extremely efficient. Due to their "depth" in the nanostructure there is a very high chance that a photon will be absorbed, and the dyes are very effective at converting them to electrons. The Ruthenium 535 bis-TBA also known as N719 or dye salt and its can sensitized up to 750 nm , is one of most efficient sensitizer in DSSC. The Ruthenium 535 also known as N3 and its is also sensitized up to 750 nm. The Ruthenium 620-1H3TBA also known as N749 or black salt and its can sensitized up to 920 nm also one of most efficient Ruthenium sensitizer. The following types of Ruthenium based dye are commonly used in DSSC design.

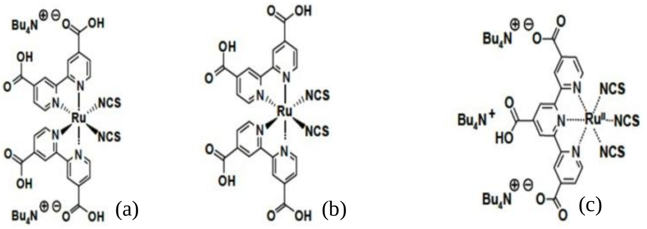

Fig 11: Ruthenium based dye: (a) Ru-535 bis-TBA;(b)Ru-535 and (c) Ru-620-1H3TBA

But one of the main problems associated with liquid based electrolytes is corrosive to metallic contacts and leakage problems. Thus, researchers have studied many different liquid and solid hole transporters. At that background, DNA based dye sensitized solar cell has been proposed as required by present DSSC scenario.

4.1 DNA Based Dye Sensitized Solar Cell

Recently, it is already reported that DNA can be a wide band gap semiconductor with non linear VI characteristic and has band gap varies from 3.75eV to 4.12eV depending upon sequence, length, orientation. Guanine rich we can't use DNA directly in molecular electronics so we heading towards hybrid technology. So several DNA hybrid materials have come some of them DNA–cetyltrimethylammonium, CTMA which is high optical quality thin film with a very low loss optical material as in [5] and also UV–VIS absorption have high transparency from 350 to about 1700 nm.

As DNA is wide band gap semiconductor as [1], so it absorb broadband optical spectrum and also act as a surface modifier, on the TiO_2 layer of DNA based dye-sensitized solar cells. A typical DNA-TiO_2 nanowire and uv-visible absorption spectra of TiO2 nanomaterials on DNA scaffolds is shown below.

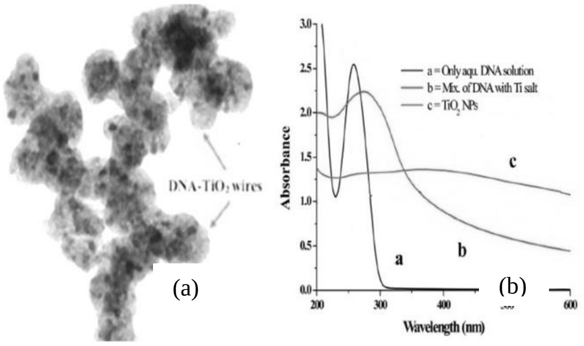

Fig 12: (a) DNA-TiO_2 nanowire; (b) uv-visual absorbance spectra.

So with presence of DNA with TiO2 nanomaterial, there is significant improvement in optical absorption, specifically in uv-visual spectra. Here DNA is used as sensitized scaffold or templates in nano building material which also gives superior of light utilization due to its symmetrical double-helix structure and improves position of Ruthenium based dye by DNA-TiO2 sensitization. A typical DNA enhanced dye sensitized solar cell energy band is shown below.

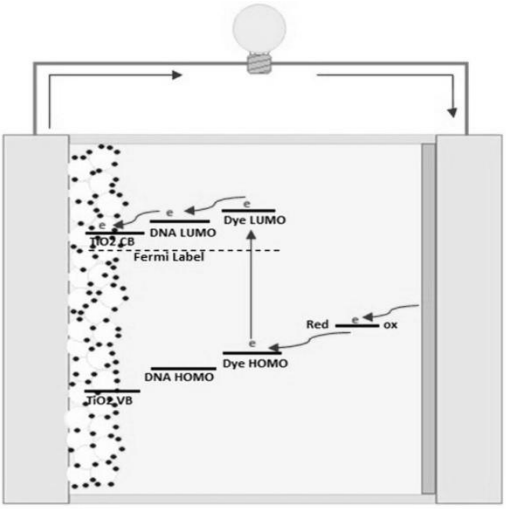

Fig 13: Energy band of DNA-TiO$_2$ based DSSC.

Here, DNA adds an extra sub energy band in between TiO$_2$ and dye band and collectively of these bands shows similar structure of Back Surface Field(BSF) as in high efficiency c Si solar cell which is further reduces carrier recombination and improves collection efficiency. The presence of DNA on the nanoporous TiO2 film enhanced the photocurrent of the device [5]. This is strong evidence that DNA molecules may have improved charge injection into the conduction band of the semiconductor due to its strong electrostatic interaction with the TiO2 nanoparticle

5. CONCLUSION

Still now, the optical loss of solar cell is major part of total loss.Dye-Sensitized Solar Cell (DSSC) is very low cost than current silicon based photovoltaic solar cell. DSSC are very efficient to absorb photon energy as it has good nanostructure depth and also the dyes are very effective at converting the photon to electrons. DNA will be one of most promising nanomaterial as it has double strand recognition and self assembly which improves optical spectrum utilization due to its symmetrical double-helix structure and nanodimensional scaffold. The presence DNA with TiO2 nanomaterial, there is significant improvement in optical absorption, specifically in uv-visual spectrum range. The actual magnitude of TiO2-DNA conductivity and its physical mechanism and charge transportation is still under debate. Beside that the effect of DNA on TiO2 dye is promising.

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