

Theory of Solar Cell (DSSC) Collection

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Abstract - Dye-sensitized solar cells (DSSCs), also known as Grätzel cells, are electrochemical devices that harness electricity by combining the physicochemical features of many materials. From a ground-breaking idea of molecule photovoltaics, these photoconversion devices have progressed to industrial production with proven record efficiencies of 14.3%. Because of their efficiency, cheap manufacturing costs, and high aesthetic attraction, DSSC devices may be made for the consumer electronics industry. This paper introduces the basic concepts behind DSSC and discusses how their efficiency might be increased for widespread use. Future work on efficiency, stability, and production that will be necessary for this technology to really represent a breakthrough in the consumer electronics sector is also mentioned. An analysis of the leading DSSC developers and their current prototypes and products is provided.

Keywords - DSSC, consumer electronics, efficiency, dye-sensitized solar cells, commercialization

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INTRODUCTION

It is widely accepted that in order to meet the significant environmental and economic concerns of the 21st century, fossil fuels, the present major but finite energy supplies, will be replaced by cleaner and cheaper renewable energy sources. Because of its potentially infinite supply, solar energy is often seen as a future power source of great potential. Therefore, efficient and cheap to produce devices are required for solar energy collection and use. Professor M. Grätzel developed the dye-sensitized solar cell (DSSC) in 1991 and it has since shown great promise as a low-cost method of capturing sunlight. Dye-sensitized solar cells (DSSCs) absorb sunlight using dye molecules adsorbed on nanocrystalline oxide semiconductors like TiO₂. Therefore, the natural light harvest in photosynpapper is mimicked by separating the light absorption and charge collecting operations. It allows us to employ inexpensive oxide semiconductors with a broad band gap in solar cells as an alternative to more costly materials like silicon or semiconductors from the III-V group. Therefore, it is possible to produce solar energy for less than \$1 per peak Watt (\$1/pW). In contrast, the current market leaders, crystalline or thin-film Si solar cells, cost >\$4-5/pW due to a global Si scarcity. In addition, a DSSC requires 40% less energy to fabricate than a Si cell.

Energy challenges emerge across disciplines as the global population rises. The ExxonMobil study estimates that in 2005, the world's energy needs were around 210 million oil-equivalent barrels per day. Today, we produce more over 300 million oil equivalent barrels per day, a 42.8% increase from

2005 levels. As of 2007 (ExxonMobil). In 2007, the Energy Information Administration projected that fossil fuels accounted for 86.4% of the world's primary energy consumption, with petroleum accounting for 36.0%, coal for 27.4%, and natural gas for 23.0%. According to the EIA (2008), the U.S. Not only should the pollution caused by burning fossil fuel be taken into consideration, but also its nonrenewable nature. U.S. EPA research suggests that burning fossil fuels accounts for more than 90% of all manmade greenhouse gas emissions (U.S. EPA, 2009). However, fossil fuels remain the most popular energy resource owing to their low cost and relative lack of technical limitations.

Over the last several decades, many alternatives to fossil fuels have emerged. However, most of them fell short of replacing fossil fuels owing to the former's widespread use, relatively high price, and associated pollution. Since 1954, scientists have learned a great deal about solar cells, one of the cheapest and safest methods to create power. Perlin, 2004 Solar cells are a kind of semiconductor device that can directly convert solar energy into electrical current. Solar cells convert light into energy by photo-generating charge carriers in a light-absorbing substance and then separating these charge carriers so they may interact conductively and transport power. Hybrid solar cells based on inorganic and organic molecules are an exciting new development in the solar cell industry.

In this project, we created a solar cell system called a Dye-Sensitized Solar Cell, which consists of a TiO₂ layer that serves as the electron carrier and an

organic dye layer that serves as the electron generator and is restored to its former condition thanks to an electron provided by the electrolyte solution. One of the biggest obstacles for solar energy is improving solar cell efficiency. The organic dye layer, or "photo sensitizer," must have properties that match those of the light spectrum accessible for the solar cell to function properly. The efficacy and cost of photo sensitizers vary because they absorb light differently. The dye sensitized solar cell was selected because to its high reported quantum efficiency and reasonable price.

LITERATURE REVIEW

Sharma, k., sharma, v. et.al (2018) Due to its cheap cost, easy preparation process, low toxicity, and simplicity of manufacture, thin-film solar cells like dye-sensitized solar cells (DSSCs) have been the subject of intensive study for over two decades. Because of their high price, little availability, and poor long-term stability, present DSSC materials still have a lot of room for improvement. Optimizing material and structural properties has increased the efficiency of existing DSSCs to as high as 12% using Ru (II) dyes, but this is still lower than the efficiency offered by first- and second-generation solar cells, such as other thin-film solar cells and Si-based solar cells, which is around 20% to 30%. This article gives a comprehensive overview of DSSCs, including their design, operation, and significant issues as well as their potential efficient materials and a quick look into commercialization.

Qian liu , et.al (2018). For use in solar cells, scientists have successfully isolated a group of natural photoactive dyes, dubbed D1-D6, from the leaves of six different plant species. UV-Vis absorption spectra, cyclic voltammetry, and photovoltaic measurements were all used to ascertain the photoelectrical characteristics of dyes. Chlorophyll was chosen as the reference dye, and its ground and excited state characteristics were computed using density functional theory (DFT) and time-dependent density functional theory (TD-DFT) in order to mathematically expose the experimental results. The visible light areas of 400-420 nm and 650-700 nm are where the experimental findings demonstrate the absorption peaks of those dyes are most concentrated, which is in agreement with the absorption spectra of chlorophyll. Solar cells sensitized with the six types of natural dyes have increasing efficiencies of photoelectric conversion as follows: D1 > D4 > D2 > D5 > D6 > D3. With an open circuit voltage of 0.58 V, a short-circuit current density of 2.64 mA cm², and a fill factor of 0.70, dye D1 performance has the greatest photoelectrical conversion efficiency (PCE) among the six natural dyes studied.

Tomás delgado-montiel, et.al (2019) Density functional theory calculations and studies were performed on ten molecules using the M06 density functional and the 6-31G(d) basis set. The molecular systems may find use as dye-sensitizers for solar

cells. Seven compounds, including one with an azomethine group in the -bridge to facilitate greater charge transfer, have been proposed after being inspired by these three molecules from the literature. Donor components include triphenylamine, -bridge components include various azomethine, thiophene, and benzene derivatives, and acceptor components include cyanoacrylic acid. The impact of the azomethine group on the -bridge was the primary focus of this investigation. We optimized the ground-state geometry and determined the highest occupied and lowest empty molecular orbitals as well as their respective energies. Time-dependent density functional theory using the M06-2X density functional and the 6-31G(d) basis set was used to calculate absorption wavelengths, oscillator strengths, and electron transitions. We evaluated the free energy of electron injection (G_{inj}). Chemical hardness, electro donating power, electro accepting power, and the electrophilicity index are only few of the chemical reactivity metrics covered in this investigation. In conclusion, the charge transfer and electrical characteristics of triphenylamine-based dyes were enhanced by the addition of azomethine in the -bridge.

Ife fortunate elegbeleye, et.al (2018) Recent years have seen a surge in research and development into dye-sensitized solar cells, which have the potential to become a competitive alternative to more traditional silicon-based solar cells. As sensitizers for DSSCs, organic and inorganic compounds have found widespread use recently. Dye sensitizers are notable for their high absorption of light in the ultraviolet, visible, and near-infrared regions of the solar spectrum. Sensitized dye molecules adsorbed on TiO₂ perform light absorption and charge separation. In this study, the UV-Vis absorption spectra of a variety of polyene-diphenyl aniline organic chromophores were analyzed by using the time dependent-density functional theory. It was possible to replicate some properties of dye molecules, such as their HOMO-LUMO energy levels, maximum excitation wavelength, excitation energies, and light-harvesting efficiencies. The findings shown that the HOMO-LUMO energy gap is decreased and the bathochromic shift is seen in dyes containing methoxy groups in the donor moiety. The findings are consistent with prior research and compare favorably.

Mohamad rodhi faiz, et.al (2018) For the purpose of Dye-Sensitized Solar Cells (DSSCs), we have theoretically investigated the electron excitation and absorption spectra of chlorophyll solution in a variety of solvents using density functional theory (DFT) and time-dependent DFT (TD-DFT). Aceton, acetonitrile, DMSO, ethanol, hexane, methanol, THF, and water were used as solvents. There has also been research into things like energy output, oscillator power, light harvesting efficiency, and electron injection. The presence of the solvents caused the investigated dye to exhibit increased light harvesting, oscillator strength, and a red shift in the absorption

spectra, as well as a decreased gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). These modifications enhance the performance of solar cells by easing charge transport processes in the nano structure of chlorophyll as a dye.

DYE-SENSITIZED SOLAR CELLS (DSSCs)

PHOTOELECTROCHEMICAL CELLS

Charge separation at the interface of two semiconductor materials is the fundamental principle behind photovoltaic solar cells. Photons are either absorbed, reflected, or transmitted when they strike a photovoltaic cell. The device's photovoltaic process is the result of photons being absorbed. As illustrated in Figure 1, the p-type semiconductor in a PV cell is responsible for absorbing the photons, and then the excited electrons are transmitted to the n-type semiconductor.

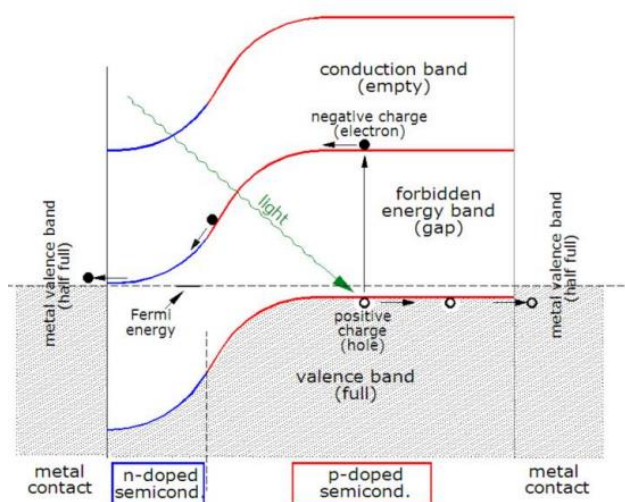


Figure 1 Band diagram of a solar cell

Electrical energy is generated when photons are absorbed by a p-type semiconductor, raising its electrons from the valence band (VB) to the conduction band (CB), and then moving them to an n-type semiconductor for use in an electrical circuit. These electrons can only flow in one way because of the potential difference at the p-n junction. A typical solar cell is seen in Figure 2. To prevent the dispersion of the incoming sunlight and optimize the absorption, a cell is often constructed from an encapsulant, which may be glass or other material that seals off the cell's components from the outside. A front contact grid, a metallic conductor that collects electrons, is the next layer. Next, the p-type semiconductor, often silicon or another material that has been doped, is put, followed by the n-type semiconductor. The metal back contact completes the circuit by covering the cell's rear end.

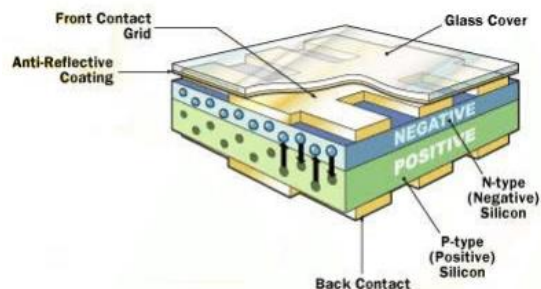


Figure 2 Common structure of a photovoltaic cell

In contrast to the previously mentioned cell, photoelectrochemical cells use a redox mechanism to convert light into electricity. The cell's electrical potential is established during this procedure. Dye-sensitized solar cells are part of this category; they date back to the early 1970s when a chlorophyll-sensitized zinc oxide (ZnO) electrode was created at the University of California. Unfortunately, the DSSCs' performance was dismal. The efficiency wasn't raised to 7% until nanoporous titanium dioxide electrodes were used by Michael Grätzel and Brian O'Regan in 1991. The development of DSSC began at this time. Therefore, a fresh chance has come up to enhance these solar cells, the design and operation of which are explained further below.

ARCHITECTURE OF A DSSC

A DSSC may be broken down into its component parts: a photoanode or working electrode (WE), a counter electrode (CE), a sensitizer (dye), and a redox mediator (electrolyte) [44] (often replaced with a solid hole transporting material (HTM)).

Transparent and conductive substrate

Two sheets of a transparent and conductive material are often used to construct DSSCs. These sheets not only serve as current collectors, but also a substrate onto which the semiconductor and catalyst are deposited. In order for sunlight to penetrate the material, a good DSSC substrate should have a transparency level of at least 80%. However, the substrate also has to have a high electrical conductivity to provide an effective charge transfer and low energy losses. Fluorine-doped tin oxide (FTO, SnO₂:F) and indium-doped tin oxide (ITO, In₂O₃:Sn) are two popular substrates. Substrates like this are made from glass (often soda lime glass) that has been coated with the chemicals discussed before. In the visible spectrum, FTO films have a transmittance of around 75%, whereas ITO films have a transparency of over 80%. While the sheet resistance of ITO films is 18 cm², that of FTO is just 8.5 cm².

Working electrode

A semiconductor oxide, such as TiO₂, ZnO, SnO₂ (n-type), Nb₂O₅, and NiO (p-type), is deposited on the aforementioned substrates to create the working electrode (WE). The energy gap in these oxides is rather large. TiO₂ is the most used oxide since it is non-toxic, inexpensive, and widely available. However, these semiconductors absorb only a little amount of light without being coated or submerged in a sensitizer, which greatly improves their efficiency. This dye is chemoattracted to the TiO₂ surface, where it forms covalent bonds by adsorption. Light absorption is greatly enhanced by the WE layer's roughness and high porosity structure, which allows many dye molecules to attach to the nanocrystalline surface of TiO₂.

Sensitizer The dye, sensitizer, or photosensitizer is what allows the cell to take in light in the first place. A dye may be made from any substance, but for best results, it should have the following qualities: If it's going to give out the light it soaked up, it has to glow. In order to absorb as much light as possible, the dye's absorption spectrum has to extend from the UV to the NIR. Lowest unoccupied molecular orbital (LUMO) should be closer to the WE surface and have a greater potential with regard to the WE conduction band than the highest occupied molecular orbital (HOMO) does. The volume of digital exchange is therefore increased.

- The redox electrolytes' HOMO should be less than the HOMO of the solvent.
- The dye has to be water repellent. The cell's stability would be compromised otherwise due to a distortion caused by the presence of water. Dye molecule aggregation on the WE oxide surface is a typical issue. Alkoxy-silyl carboxylic acid group and co-absorbents like chenodeoxycholic acid (CDCA) are all examples of anchoring groups that may be inserted between the dye molecule and WE to prevent this from happening. Limiting the recombination process and making bonds more stable are also effects of preventing aggregation.

Electrolyte

The electrolyte consists mostly of a solvent or ionic liquid, additives, and cations, as well as a redox couple (such as I⁻/I₃⁻, Br⁻/Br₂⁻, SNC⁻/SCN₂ or CO(II)/Co(III)). The following are characteristics of an excellent electrolyte: The oxidized dye must be regenerated by the redox couple. It has to be chemically, thermally, and electrochemically stable.

- The DSSC shouldn't be corroded by the solvent or the electrolyte's various components. It has been shown to have a high efficiency in the case of I⁻/I₃⁻, but it presents substantial constraints due to corrosion of the glass. As a result of photodegradation and dye desorption, it is also very volatile and has an impact on the cell's long-term stability.
- Electrolyte absorption spectra and dye absorption spectra must not cross. A good connection between the WE and CE, efficient diffusion of charge carriers, and increased conductivity may all result from selecting the right electrolyte.

Counter Electrode (CE)

Platinum (Pt) or carbon (C) is often used in the fabrication of the counter electrodes. The CE's job is to catalyze the redox couple's decomposition. Platinum-composed CEs have a high efficiency but they are problematic since Pt is costly and difficult to come by. Wu et al. provide a summary of a variety of alternatives that have been produced, including carbon, carbonyl sulfide, and alloy CEs.

3.3. WORKING PRINCIPLE OF A DSSC

A dye-sensitized solar cell's operation may be broken down into four stages: light absorption, electron injection, carrier transport, and current collection. The primary function of a DSSC device is to convert solar light into electricity without undergoing any kind of irreversible chemical change. The kinetics of DSSCs is vast and complicated because it involves the study of the transport of electron-hole charges over several poorly defined surfaces. The kinetic processes at play in these cells are shown in Figure 3.

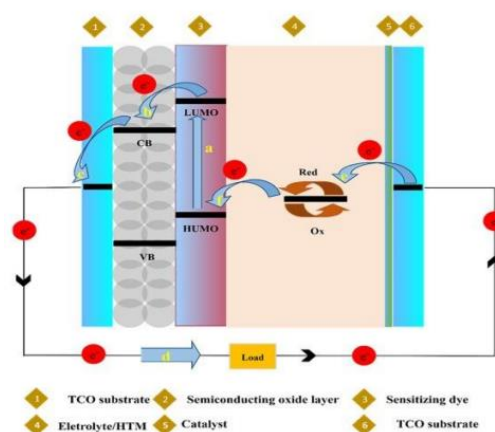
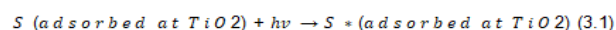
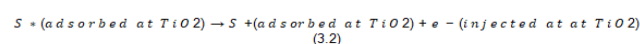


Figure 3 Diagram of the operation of a DSSC. The processes that take place are (a) photo-excitation, (b) injection, (c) transport, (d) conduction, (e) diffusion and (f) regeneration

Interfacial electron transport mechanisms are the basis of the working principle. A photon ($h\nu$) is absorbed by the sensitizer or dye (S) and fixed on the semiconductor, which transitions to an excited state (S^*) when incoming light strikes the photoelectrode. In other words (equation):

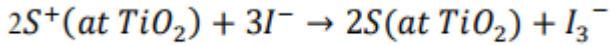
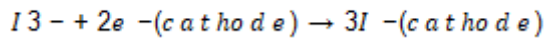


Dye's excited state (S^*) may release or inject an electron into the conduction band (CB) states of TiO₂ to form S^+ oxidative species (equation).

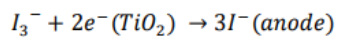
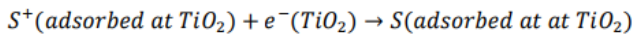


Once in the TCO layer, the porous semiconductor linked network of TiO₂ nanoparticles aids in the transport of electrons. Electrons in the TCO layer are sent to the CE through the external circuit. The electrolyte absorbs this transferred electron by diffusion, converting I₃ to I (equation 3.3). Dye

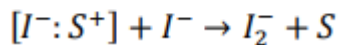
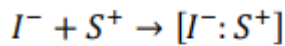
regeneration occurs after I⁻ is formed, as shown in equation 3.4, when the previously S⁺ oxidative species react with the produced I⁻ to produce a non-excited dye and I₃⁻ once again, completing the current cycle.



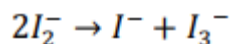
Recombination processes are what happen when this happens, and they lead to inefficiency. The injected electrons in the TiO₂ CB may either be transported to the oxidized dye (equation) or to the I₃⁻ ions that are located near the semiconductor's surface (equation):



Reactions seem to proceed sequentially in equation, while the mechanism for the reduction of dye cations is still up for discussion.



where 3.7 is brisk and 3.8 is slow. After this stage, the process becomes murky, and other explanations are entertained. Regeneration processes, as shown in equation 3.8, require the presence of a second iodide ion (I⁻) interacting with a [I⁻:S⁺] complex. However, the presence of a thiocyanate (SCN⁻) ligand in the dye is essential for this reaction to take place. The intermediate complex is a mystery when this ligand is absent. Diiodide, I₂⁻, is released from the dye molecule upon contact with the second iodide. Then, the diiodide radicals become unbalanced and split into iodide and triiodide.



In the presence of sunlight, the difference between the quasi-Fermi level and the redox potential of the redox pair in the electrolyte provides the driving force. Injecting (equation) and regenerating processes (forward reactions) must have a kinetic advantage over recombination (back-reactions) if excellent efficiencies are to be achieved. Figure 4 is a visual representation of the many processes and time scales. Due to the relative slowness of photoelectron recombination and dye regeneration, the DSSC idea is viable.

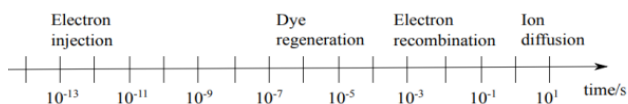


Figure 4 Time scale of the different processes in a DSSC

The sensitizer's ability to absorb light is also crucial to DSSCs' method of operation. An electron is displaced from the most filled molecular orbital (HOMO) to the least filled orbital (LUMO) when the dye absorbs light. The electronic transfer must take place between the dye's orbitals and the semiconductor's energy bands, therefore their relative location is crucial.

THERMODYNAMICS OF DSSCS

Concentration gradients created during charge separation processes aid diffusion, the primary mechanism for charge transfer in DSSCs. Redox potential differences between species at the reaction interfaces (TiO₂/dye/electrolyte) are responsible for charge separation in DSSC from a thermodynamic perspective. In order to encourage the transfer of an electron excited by light from the LUMO of the dye to the conduction band of TiO₂, the potential presented by the dye must be less than the potential of the TiO₂ conduction band. Like the HOMO level, the electrolyte's potential (3I⁻/I₃⁻) must be higher than the HOMO level of the dye. Cell power is another thermodynamic variable. The power is associated with both the process of charge separation and the resulting photovoltage, which is the energy gap between the electrodes. Therefore, DSSC maximum power is equal to the electrolyte redox potential minus the TiO₂ Fermi level. The difference in energy between the dye's HOMO and LUMO states also governs the cell current. If, after being exposed to 1000 W/m² of light at 25 C, the cell produces at least 20 mA/cm² it is considered efficient and competitive in the market.

DSSC PHOTOVOLTAIC PARAMETERS

To evaluate the relative performance of various DSSCs, researchers may now use a variety of metrics that are independent of the devices' specific operating circumstances.

Conversion efficiency

An essential aspect of a solar cell's characterization is its energy conversion efficiency. Connecting a solar cell to an electrical circuit and measuring the resulting power output is how we define "conversion efficiency." According to the total solar power incident on the cell, P_{in}, 100 mW/cm² for air mass (AM) 1.5, the overall solar conversion efficiency of DSSC, is defined by the short-circuit current density, J_{sc}, the open-circuit photovoltage, V_{oc}, and the cell fill factor, FF. The phrase provides it:

$$\eta = \frac{P_{max}}{P_{in}} = \frac{J_{sc} \cdot V_{oc} \cdot FF}{P_{in}}$$

Open-circuit voltage, V_{oc}

Maximum voltage produced by a solar cell while no current is flowing is called the open circuit voltage (V_{oc}).

short-circuit current, I_{sc}

When the voltage across a solar cell is zero, the maximum current, I_{sc} , flows through the cell. Short circuit current density, J_{sc} , is more often used since it does not rely on the size of the solar cell. In a perfect solar cell, the light-generated current density is equivalent to the short-circuit current density. In reality, the current density is a function of the amount of sunlight reaching the cell as well as the cell's capacity to absorb and reflect light.

Fill factor, FF

Both the solar cell's maximum voltage and current have already been specified. However, the power output of the solar cell is zero in both operational conditions. The fill factor is calculated by dividing the solar cell's maximum power output (P_{max}) by the sum of its open circuit voltage (V_{oc}) and short circuit current (J_{sc}). Normal FF values range from 0.40 to 0.80. There isn't much space for growth, thus it's not a really intriguing study parameter. It should be made clear, however, that the FF is affected by the total series resistance of the cell, which includes the sheet resistance of the substrate and counter electrode, the electron transport resistance through the working electrode, the ion transport resistance, and the charge-transfer resistance at the counter electrode.

I-V curve

Current-voltage characteristics, or I-V for short, are a graphical representation of how a solar cell works, as seen in Figure 5. Open circuit voltage is the voltage across an open circuit, while short circuit current is the current across a short circuit. From zero volts to V_{oc} , the current is almost constant up to a maximum voltage of V_{max} , and then it drops off sharply. The power, $P = V I$, may be determined at any point on the curve.

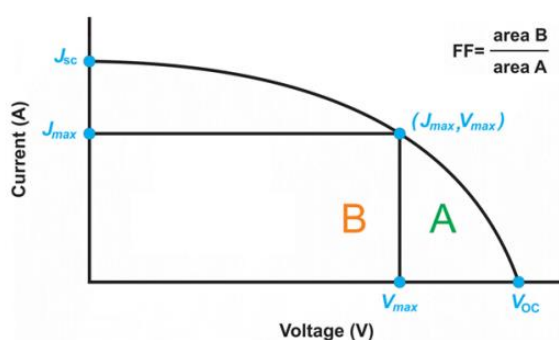


Figure 5 I-V curve used to evaluate cells performance

CONCLUSIONS

The concept of DSSCs, conceived by Michael Grätzel in the 1990s, has gone from science fiction to reality in a span of less than 30 years. Despite this development, the fundamental principles of photoelectrochemical operation have remained intact; instead, research has focused on improving the use of dyes, redox shuttles, and various architectural methods to increase efficiency. For extensive market acceptance, a PV technology must be effective, stable over time, and reasonably priced. The certified efficiency of DSSCs has reached 14.3 percent [74], and they have functioned admirably in outdoor testing over many years and under continuous illumination for more than 20,000 hours [106, 108]. The cost of both raw materials and labor is expected to fall as solar cells gain in popularity, manufacturing increases, and production efficiency increase. All of these separate technologies are expected to coexist in the future PV industry. This paper's author concludes that as DSSCs develop, they should give more weight to complementary relationships than to competitive ones. Success will come from narrowing down on the technology's final use rather than adopting a broad approach.

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