DESIGN, OPTIMISATION AND COMPARATIVE STUDY ON LEAD FREE PEROVSKITE SOLAR CELL

USING SCAPS-1D

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PROJECT REPORT APPROVAL

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DECLARATION OF CANDIDATE

We hereby declare that the undergraduate research work reported in this thesis has been performed by us under the supervision of Professor Dr. Md. Fokhrul Islam and this work has not been submitted elsewhere for any purpose (except for publications)

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DEDICATION

We dedicate our thesis work to our parents and teachers. A special feeling of gratitude to our loving parents. In addition, we express our deep gratitude towards our respected thesis supervisor Professor Dr. Md. Fokhrul Islam.

We also dedicate this thesis to our many friends who have supported us throughout the process. We will always appreciate what they have done.

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“*In the name of ALLAH, Most Gracious, Most Merciful*”

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ABSTRACT

Perovskite solar cells have gotten a lot of attention in recent years because of their appealing characteristics, such as higher efficiency in higher spectrum range, low production costs, ease of fabrication, and steadily improving system efficiencies. The development of new manufacturing methods, materials, system architectures, and improved stability have been the subject of research efforts. In this study we have analyzed two optimized cell models which have been simulated in SCAPS-1D and have compared the characteristics between them.

The optimization was set to the thickness and doping concentration(NA) of the perovskite layer, electron affinity of the ETM(Electron transporting medium). We used the whole standard spectrum to find the best possible range to get high QE. As different materials are being tested to be used in perovskite solar cell recently, we have switched two substances in the ETM keeping in mind about their optoelectronic qualities and production cost. Then a comparative analysis has been done depending on the I-V and QE characteristics of this two models. The open circuit voltage and the short circuit current have also been taken into account alongside the FF% and conversion efficiency.

CHAPTER ONE

INTRODUCTION

1.1 GENERAL

The world is currently craving for RE (renewable energy) and from those energies the energy that has the most appeal is Solar Energy. It's not only for the availability or the infinite amount of the source but also the easiest one to convert or bend to human will. Bangladesh is one of the leading countries who are using solar energy for making more than 1GW of solar energy. Bangladesh is a country of 147,570 km^2 with a population of 159 million. The country has shown tremendous growth in recent years, and has attained an average gross domestic product growth rate of 6 per cent. Booming economic growth, rapid urbanization, and expanding industrialization and development have increased the country's demand for electricity. It is recognized that energy is the key ingredient to alleviate poverty and to improve the socioeconomic condition of the people of Bangladesh. The vision of the Government is to make electricity available for all by 2021. In order to fulfill the vision, the Government has given topmost priority to the power sector and has prepared short-, medium- and long-term power generation plans using gas, coal, duel fuel, nuclear and renewable energy resources. Renewable energy will play a vital role in meeting the demand for electricity, especially in the off-grid areas of the country. The Government has set a target to generate 5 per cent of the total electricity supply from renewable energy resources by 2015 and 10 per cent by 2020. To achieve this goal, the Government has taken up a number of renewable energy programs.

1.2 LITERATURE REVIEW

Energy is defined as capacity to produce an effect to do work. Energy has been an important component to meet the day to day needs of human beings. Human society require increasing amount of energy for industrial, commercial, domestic, agriculture, and transport uses. Different forms of energy are defined as primary and secondary energy, commercial and noncommercial energy, renewable and nonrenewable energy. Renewable energy is obtained from natural sources. These resources can be used to produce energy again and again eg. Solar energy, wind energy, tidal energy etc. Nonrenewable resources cannot be replaced once they are used eg. Coal, oil, gas etc. these energy resources are limited and would be exhausted within prescribed period of time. Primary energy refers to all types of energy extracted or captured directly from natural resources. Primary energy can be further divided into two parts namely renewable and non-renewable energy. Primary energy is transformed into more convenient form of energy such as electricity, steam etc. these form of energy are called secondary energy. Energy that is available in the market for a definite price is known as commercial energy. And Solar Energy is molded to a new form of commercial energy in current days.

Solar energy is the Sun's radiant light and heat harnessed across a variety of ever-changing technologies, such as solar heating, photovoltaic, solar thermal energy, solar architect molten as lt power plants and artificial photosynthesis. It is an important source of renewable energy, and its systems, depending on how they absorb and transmit solar energy or transform it into solar electricity, are broadly defined as either passive solar or active solar. In order to harvest electricity, active solar strategies include the use of photovoltaic devices, concentrated solar power and solar water heating.

1.3 PROBLEM STATEMENT

The world lacks safe, low-carbon, and cheap large-scale energy alternatives to fosil fuels. ... The problem that dominates the public discussion on energy is climate change. A climate crisis endangers the natural environment around us, our wellbeing today and the wellbeing of those who come after us. The world is losing its natural mineral fuels day by day. So, its high time we think about other alternatives. Here comes the solar energy. It is free and unlimited. Sunlight have uv rays and many other electromagnetic rays which we can convert into electric power. This power is free and there is no pollution. But we face problems in here too. The problems are following:

1. Cost

The initial cost of purchasing a solar system is fairly high. This includes paying for solar panels, inverter, batteries, wiring, and the installation. Nevertheless, solar technologies are constantly developing, so it is safe to assume that prices will go down in the future.

2. Weather-Dependent

Although solar energy can still be collected during cloudy and rainy days, the efficiency of the solar system drops. Solar panels are dependent on sunlight to effectively gather solar energy. Therefore, a few cloudy, rainy days can have a noticeable effect on the energy system. You should also take into account that solar energy cannot be collected during the night. On the other hand, if you also require your water heating solution to work at night or during wintertime, thermodynamic panels are an alternative to consider.

3. Solar Energy Storage Is Expensive

Solar energy has to be used right away, or it can be stored in large batteries. These batteries, used in off-the-grid solar systems, can be charged during the day so that the energy is used at night. This is a good solution for using solar energy all day long but it is also quite expensive.

In most cases, it is smarter to just use solar energy during the day and take energy from the grid during the night (you can only do this if your system is connected to the grid). Luckily your energy demand is usually higher during the day so you can meet most of it with solar energy.

4. Uses a Lot of Space

The more electricity you want to produce, the more solar panels you will need, as you want to collect as much sunlight as possible. Solar PV panels require a lot of space and some roofs are not big enough to fit the number of solar panels that you would like to have.

An alternative is to install some of the panels in your yard but they need to have access to sunlight. If you don’t have the space for all the panels that you wanted, you can opt for installing fewer to still satisfy some of your energy needs.

5. Associated with Pollution

Although pollution related to solar energy systems is far less compared to other sources of energy, solar energy can be associated with pollution. Transportation and installation of solar systems have been associated with the emission of greenhouse gases.

There are also some toxic materials and hazardous products used during the manufacturing process of solar photovoltaic systems, which can indirectly affect the environment.

1.4 OBJECTIVE OF STUDY

The objectives of this study are to:

- Initial cost of establishing a solar panel is very high due to its materials are very expensive. We are up to reducing the manufacturing cost of solar cell.
- Besides reducing the manufacturing cost we are also focusing on efficiency. We are trying to keep the efficiency of solar panel with respect to other high quality solar cells.
- Most of the solar cells are not stable in bad weather. Due to humid weather the solar panel loses its strength and stability. We are also focusing on this side and our solar cell will survive in bad weather as well as humid condition.
- We're trying to compare between two models to see which is best suited.
- Our one of the main concern also is to save mother earth. As we are saving its fossil energy, we have to save its environment too. Most of the solar cells are made with harmful toxic chemicals like lead and etc. We are up to making a lead free solar cell which will be more convenient.

1.5 SCOPE OF STUDY

There were several tasks that were necessary to be done in order to complete the before mentioned objectives which are given below:

1. Establishing the appropriate instruments for conducting research on the perovskite solar cell.
2. Simulating the real life issue in SCAPS-1D and checking the efficiency points
3. Comparing the theoretical simulation with the real life situation.
4. Comparing with other models by simulating it in SCAPS-1D and check the efficiency and other parameters.

CHAPTER TWO

Solar Energy and Solar Cell

2.1 INTRODUCTION

Energy is defined as capacity to produce an effect to do work. Energy has been an important component to meet the day to day needs of human beings. Human society require increasing amount of energy for industrial, commercial, domestic, agriculture, and transport uses. Different forms of energy are defined as primary and secondary energy, commercial and noncommercial energy, renewable and nonrenewable energy. Renewable energy is obtained from natural sources. These resources can be used to produce energy again and again eg. Solar energy, wind energy, tidal energy etc. Solar photovoltaic energy is the energy of the future. It can resolve a lot of the ecological and energy problems of the world. The energy sources of our planet are running out. Petrol, gas, and coal are available in limited amounts. Utilization of such resources, however, harms the environment – gas emissions of greenhouse effect being the main reason for global warming. Moreover, the energy consumption is increasing. Till 2030, a 50% increase in energy needs is expected. A possible limitation of electricity consumption would mean deteriorating of lifestyle. Therefore, existing without electrical energy is practically unthinkable. Besides the problems related to limited amounts of energy resources and ecology issues, many people are experiencing the attitude of brutal negligence and shady pricing policy of local utilities and energy companies. Frequent power outages, continually changing and often

Fig 2.1 : Solar Energy

Incomprehensible tariffs, and pricing of electricity, oil, and natural gas are gradually becoming common. Also, it is proved that utilities have no short-term economic benefit to prevent infrequent large-scale power cuts and cascading failures in power grids. Naturally, they do little to none to improve customer satisfaction in that direction. What is more, the uncertain geopolitical and ecological situation on the planet forces many people to embrace the idea of self-reliance and seek ways to become more energy independent even at any cost. In this situation, renewable power sources are the only solution. Solar generators, wind generators, and biofuel products are by all means the Technology of the Future. Utilization of inexhaustible natural resources for energy production is a necessity standing in front of the whole of humanity.

2.2 Solar Energy

The earth receives the solar energy in the form of solar radiation. These radiations comprising of ultra-violet, visible and infrared radiation. The amount of solar radiation that reaches any given location is dependent on several factors like geographic location, time of day, season, land scope and local weather. Because the earth is round, the sun rays strike the earth surface at different angles (ranging from 0° to 90°). When sun rays are vertical, the earth's surface gets maximum possible energy. Most of the part of India receives 4 to 7 kWh of solar radiation per square meter per day. India receives solar energy equivalent more than 5000 trillion kWh per year.

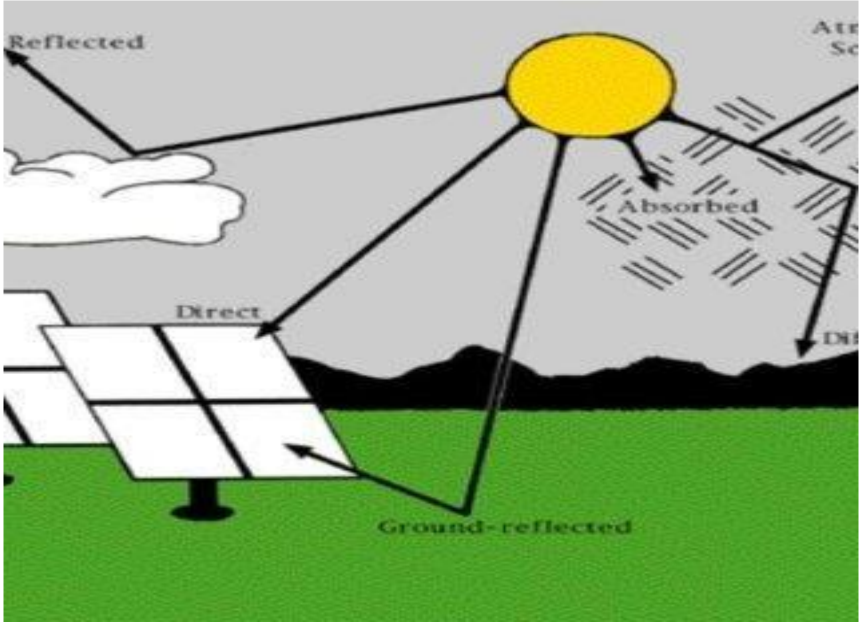


Fig 2.2 : Solar Energy and Radiation

2.2.1 Advantages of Solar Energy

For the user:

1. A well-developed, proven, and reliable technology.
2. No moving parts and little maintenance.
3. No fuel needed for operation.
4. An easy and quick mounting, especially grid-tied systems.
5. Off-grid Solar Energy systems are capable of producing electricity anywhere in the World.
6. Photovoltaic systems generate more energy than they consume – the energy invested in solar panels can be returned in 2 to 7 years, depending on the location and solar system type.
7. Photovoltaic add value to the building where they are installed.
8. Energy independence.
9. Satisfaction from achieving more energy security and bringing family comfort during a power outage.

For the environment:

1. Solar Energy systems help for reduction of carbon dioxide emissions, thus minimizing the greenhouse effect.
2. Solar Energy systems reduce environmental pollution and do not cause any environmental risks – oil spills, nuclear disasters, global warming.
3. Solar Energy save the scarce resources available in the bowels of the Earth.

4. Solar Energy can be recycled – there are various technologies for recycling panels after they are worn out or damaged; solar cells, glass, aluminum frames can be either recycled or reused.

2.2.2 Worldwide Popularity of Solar Energy

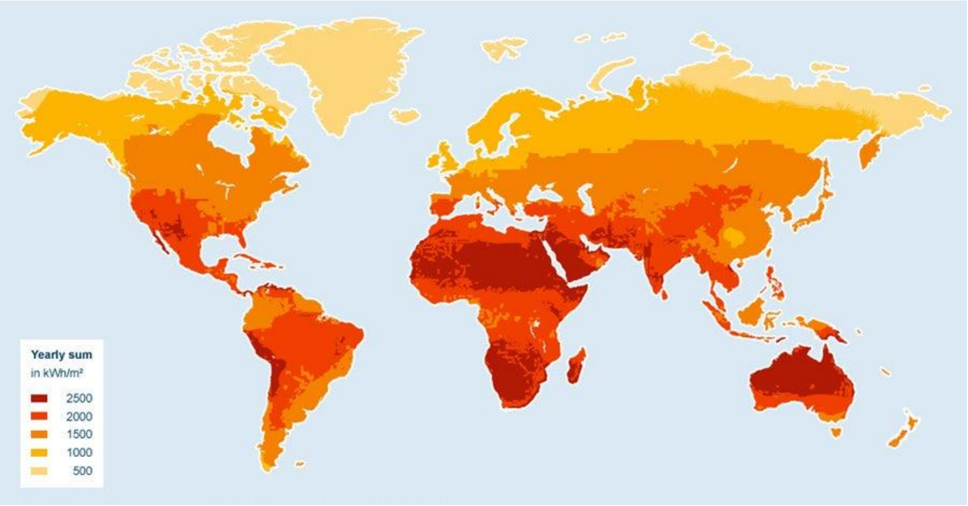


Fig 2.2.2.1 : Worldwide Popularity of Solar Energy

They stimulate sensible and economical energy use. Solar energy gives us renewable energy. It is a popular technology and advertise renewable energy successfully. The shining of the sun is more reliable and more predictable than the wind. Also, annual values of radiation are relatively constant per given area. As the surface area of earth is constant. So, the space for establishing solar panels will be constant too. It is a very wise decision to implant solar panels on the roof of buildings and structures. The energy of the sun is uniformly distributed on the surface of the Earth. The solar power technology performs well both in countries located far from the equator and in tropical areas. Installation of photovoltaic fosters research and development of a technology of the future. Investing in solar power helps achieve energy efficiency and decrease the energy dependence from other countries. Though initial cost is high, it will cover up over the time. The cost of solar power systems is decreasing, and their performance is increasing as a result of: Increased efficiency of PV cells and panels. Development of thin-film technologies. Further development of alternative coatings. Improved performance and higher production appliances for crystalline silicon solar cells and panels. Improved features and mass production of PV system components.

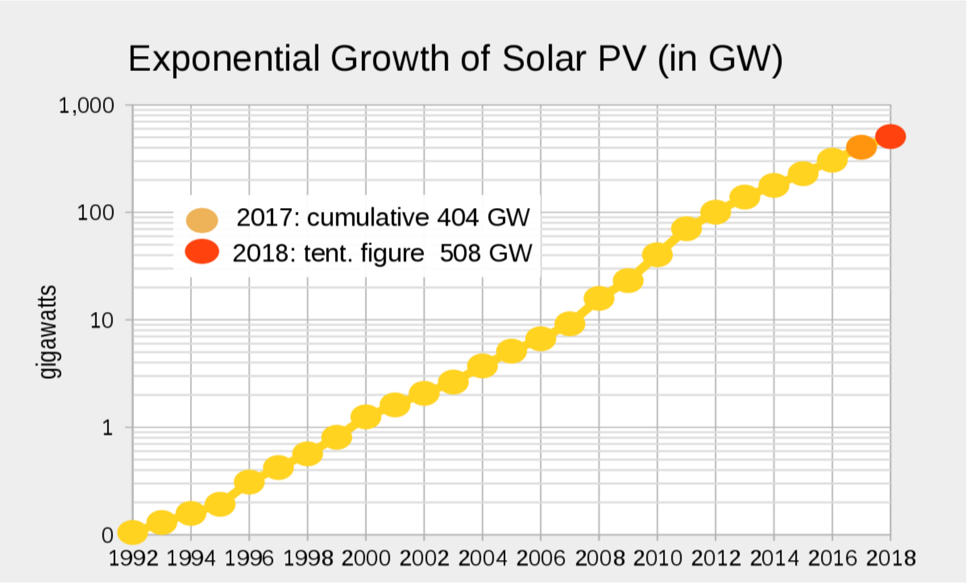


Fig 2.2.2.2 : Growth rate of Solar Energy usage

It represents a fast-growing market everywhere in the world. The usage of Solar panels is growing rapidly in world market. Now a days, in cities and villages, solar energy is gaining popularity. In the distant places far from cities, where electrical energy has not reached yet. Solar energy can be a great solution. In the hill-tract areas, where implementing substation and distribution system, individual solar panels can be a great solution.

2.2.3 Drawbacks of Solar Energy

The overall initial cost of system buying and installation is still high. Compared to the efficiency of wind power generators, the efficiency of solar power systems is lower. In other words, the area needed to produce certain power is much larger if you use photovoltaic instead of wind generators. However, the efficiency of solar panels is not as location-sensitive as in wind turbines. A solar power system can be deployed at almost any place. This is not valid for wind power, however, which is advantageous mostly in coastal areas and areas with relatively high wind speed. Also, thanks to the constantly decreasing prices of solar panels and other components of the solar panel system, solar power gradually becomes competitive with wind power. The sun is not always available as a source of energy. This means that for periods of ‘sun outage’ you need an additional system for electricity storage. Solar-generated electricity is still more expensive than the electricity supplied from a utility grid unless you live in a remote area where connecting to a utility grid would cost you a fortune. PV systems make solar electricity more affordable than it was 20-30 years ago, but prices remain relatively high. Nevertheless, in the last few years, prices of solar photovoltaic panels have dropped 80% on average, and they are continuing to decrease. Photovoltaic systems are not recommended for heating. For heating, you should use a solar thermal system. Another option is propane or natural gas. High costs of PV systems are concentrated in a substantial initial investment. Often the biggest problem is to find initial funding. After you install your PV system, it is nice to feel independent from the utility grid or to see your monthly electricity bills going down. Buying a PV system is actually like paying your electricity bills in advance for years ahead, and the point is to avoid the essential burden of high initial costs. Thus, finding a suitable source of financing is essential. Solar electric systems only produce power when the sun is shining. Therefore, something should be done with the electricity produced – it should be either consumed right away, or exported to the grid (in grid-tied systems), or stored in a battery for later use (in off-grid systems). For people connected to the grid, usually the decision to purchase a photovoltaic system is based on cost-saving – reducing their monthly bills by selling power to the utility. For people living in remote areas, far from any utility infrastructure, the decision to purchase a PV system is not determined by any cost-saving reasons but is a matter of securing a normal life instead.

2.3 Solar Cell

A solar cell is nothing but a PN junction diode under light illumination. Sun light can be converted into electricity due to photovoltaic effect. Sun light composed of photons (packets of energy). These photons contain various amount of energy corresponding to different wave lengths of light. When photons strike a solar cell they may be reflected or absorbed or pass through the cell. And in further creates energy surge to store.

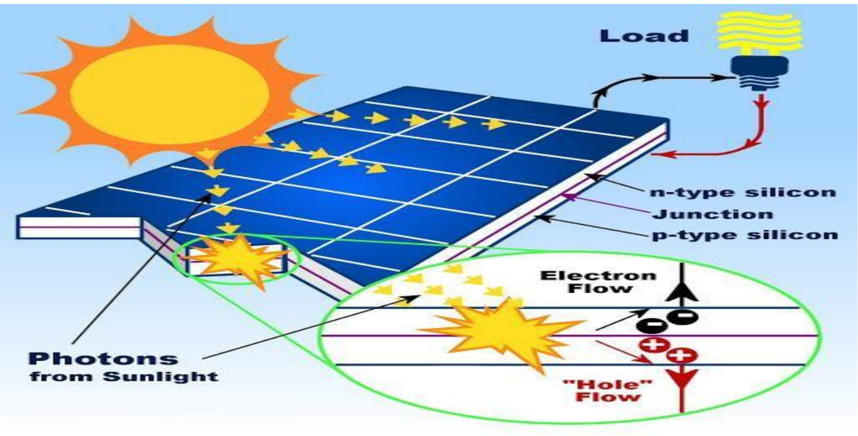


FIG: 2.3.1 Photovoltaic Cell

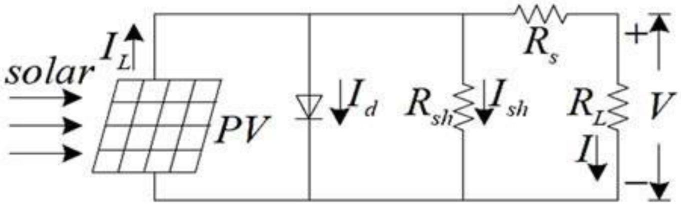


FIG: 2.3.2 Solar Panel Connection Circuit

Solar cells are devices that convert light into electricity. They are called "solar" cells because most of the time, the most powerful source of light available is the Sun, called Sol by astronomers. Some scientists call them photovoltaic which means, basically, "light-electricity." A solar panel is a collection of solar *cells*. Lots of small solar cells spread over a large area can work together to provide enough power to be useful. The more light that hits a cell, the more electricity it produces, so spacecraft are usually designed with solar panels that can always be pointed at the Sun. The circuit of the solar panel is as simple as it can get. A panel board is directly connected to the circuit that goes to the voltage storage.

2.3.1 Types of Cells

A glance at the recent literature shows that many different solar cell designs and materials are being studied. This situation is common in the early stages of technical development, when many different approaches are explored. Incidentally, terrestrial use of cells to produce power is quite recent, even though the photovoltaic effect has been known since 1839. Silicon solar cells were first described in print in 1954, and solar cells have been used on most of the spacecraft launched since then. Cells for use in space are not discussed in this book because the hostile conditions those cells must withstand, together with the extreme reliability demanded, make the space cells far too costly and specialized for terrestrial use. Although the details involve concepts of solid-state physics, chemistry, and

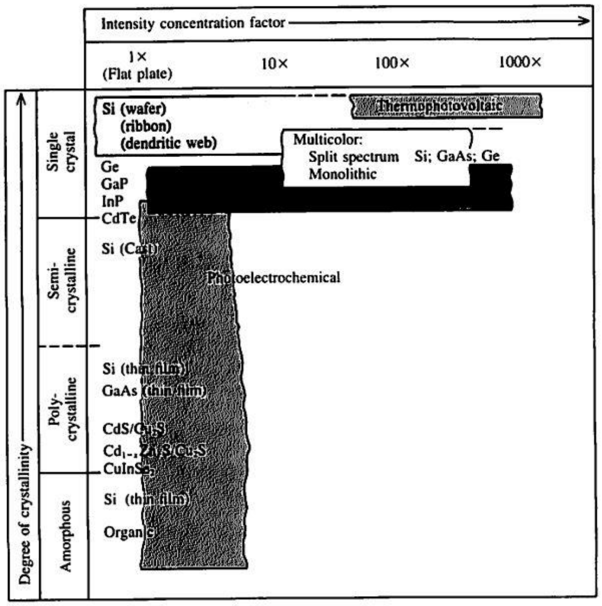


Fig 2.3.1 : Types of solar cells, arranged according to degree of crystallinity of the semiconductor and degree of sunlight concentration used

materials science, some very simple observations underlie the different types of solar cells: Because silicon has been used so extensively for integrated circuits, its technology is well developed and it is natural choice for use in solar cells now, while other approaches are being developed. Making thin-film or polycrystalline cells instead of single-crystal cells, which require extensive heating and careful crystal growth and slicing, may be economical in terms of both monetary cost and energy expended in the production process. Since focusing lenses and mirrors cost much less per unit area than do most semiconductors, it can be cost-effective to use "concentrator" systems in which sunlight is focused onto relatively small semiconductor cells. Since cells can be designed to work particularly well with light of one wavelength, it may be economical to split the spectrum and direct different portions onto cells optimized for those spectral components ("split spectrum" or "multicolor" cells). Since both available sunlight and the demand for energy fluctuate, cells providing inherent energy storage by electrolysis within the cell may be attractive ("photo electrochemical" cells). The cell types shown in Fig are arranged according to material and form of the semiconductor used and the degree of sunlight concentration employed. Some characteristics of the starting material or cell design are also indicated. The cells produced in greatest quantity have been made of single-crystal silicon, and used without sunlight concentration (upper left corner, Fig. Silicon cells have been made of wafers sawed from large single-crystal ingots, and from thin ribbons or thin webs of silicon that do not require slicing. Of the many other single-crystal cell materials that have been studied, the compound semiconductor gallium arsenide has been most used in experiments because of its high efficiency and its ability to operate at high temperatures. Concentrator cell systems have been made with both silicon and gallium arsenide. Concentrator cell configurations differ from those for non-concentrator use ("flat-plate" cells); concentrator cells must withstand higher temperatures and must have lower resistive losses because of their relatively higher cell currents. Since the split-spectrum cells involve several cells, one expects that to achieve low system cost such cells will be used initially with concentrating lenses or mirrors. Another concentrator cell involving spectral alteration in the interest of high efficiency is the "thermo photovoltaic" cell, which is illuminated by relatively long wavelength radiation from plate heated by concentrated sunlight. Most cells employ so-called/»> junctions, that is, two adjacent regions of semiconductor such as silicon that contain different impurities within them so they have different electrical characteristics. An alternative structure is the Schottky-barrier cell, in which thin, fairly transparent metal film replaces one of the semiconductor regions of the pn -junction cell. Another promising cell design contains in addition very thin insulating region between the metal and the semiconductor, forming the "metal-insulator-semiconductor" (MIS) or "metal-oxide-semiconductor" (MOS) structure. Polycrystalline cells generally have lower production and material costs than do conventionally made single-crystal cells. Alternatives to the conventional methods of making single-crystal ingots have been developed, as will be discussed . These include the edge-defined film-fed growth (EFG) and dendritic web cells. Thin-film cells, in which semiconducting film is deposited on substrate, include commercial cadmium sulfide cells, which actually have pn junction between layers of cadmium sulfide and copper sulfide, and cells made of thin films of amorphous semiconductors. Experimental cells made from organic constituents are also under investigation. Studies predict that it will be possible to make thin-film cells that are efficient and inexpensive enough to become the cells of choice for many terrestrial applications.

2.3.2 Solar Cell materials

Solar cells are typically named after the semiconducting material they are made of. These materials must have certain characteristics in order to absorb sunlight. Some cells are designed to handle sunlight that reaches the Earth's surface, while others are optimized for use in space. Solar cells can be made of only one single layer of light-absorbing material (single-junction) or use multiple physical configurations (multi-junctions) to take advantage of various absorption and charge separation mechanisms.

Solar cells can be classified into first, second and third generation cells.

The *first generation* cells—also called *conventional, traditional* or *wafer-based cells*—are made of crystalline silicon, the commercially predominant PV technology, that includes materials such as polysilicon and monocrystalline silicon.

The *second generation* cells are thin film solar cells, which include *amorphous silicon, CdTe* and *CIGS* cells and are commercially significant in utility-scale photovoltaic power stations, building integrated photovoltaics or in small stand-alone power system.

The *third generation* of solar cells includes a number of thin-film technologies often described as emerging photovoltaics—most of them have not yet been commercially applied and are still in the research or development phase. Many use organic materials, often organometallic compounds as well as inorganic substances. Despite the fact that their efficiencies had been low and the stability of the absorber material was often too short for commercial applications, there is a lot of research invested into these technologies as they promise to achieve the goal of producing low-cost, high-efficiency solar cells.

2.4 WORK PROCESS & ENERGY CONVERSION OF A SOLAR PANEL

When photons strike a solar cell they may be reflected or absorbed or pass through the cell. When solar radiation is absorbed in PN junction diode, electron-hole pairs (EHP) are generated. Electron hole pair (EHP) generated in depletion layer. Electrons of EHP will be repealed towards N side because of electric field and holes of EHP will be repealed towards P side because of electric field. Electron hole pair (EHP) generated in quasi neutral region. In this region, the electron and holes of EHP will wander around in the region randomly. There is no electric force to guide them in any direction. Minority carriers of P and N regions. The minority carrier near the depletion region will also get direction by electric field.

In this way there will be increase of positive charge at P side and increase of negative charge at N side. This build up of positive and negative charge causes a potential difference to appear across the PN junction due to light falling on it. This generation of photo voltage is known as photovoltaic effect.

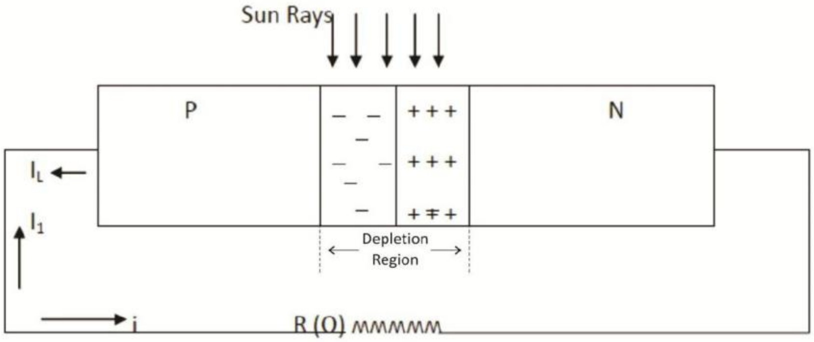


Fig: 2.4 Photovoltaic cell performance

Consider a PN junction with resistive load as shown in figure. When solar cell is illuminated, electron hole pair is generated in the depletion region. This electron hole pair when separated from each other across junction then a current (IL) flows in external circuit by photovoltaic effect. This photo current (IL) produces a voltage drop across resistive load and this voltage will forward bias the PN junction. Forward bias voltage produces forward current (I1).

So the net current will be, I = IL – I1

$$\mathrm{I} = \mathrm{I(L)} - \mathrm{I(0)}[\exp\left(\frac{ev}{kT}\right) - 1]$$

For short circuit

When R=0 and V = 0 then I1 =0 so I = IL = ISC

Power delivered to load- P= V.I

For maximum power delivered to load, dP/dV=0

$$1 + \frac{\mathrm{I(L)}}{\mathrm{I(0)}} = \exp\left(\frac{e.Vm}{kT}\right) . [\ 1 + \frac{e.Vm}{kT}\ ]$$

Where Vm is the voltage which produces maximum power

Maximum Current -

If we put the value of Exp (e.Vm/kT) from the equation we get the maximum value of Current (Im)

Maximum Power:

the maximum power is obtained by multiplying Vm and Im

$$\mathrm{Pm} = \mathrm{Vm.Im} = Vm\frac{e.Vm.(IL+Io)/kT}{1+eVm/kT}$$

CHAPTER 3

PEROVSKITE SOLAR CELL

3.1 Perovskite Materials

Basic Structure

A perovskite is a material with the same crystal structure as the first-discovered perovskite crystal, calcium titanium oxide. ABX3 is the chemical formula for perovskite compounds, where A is **an organic cation - methylammonium ($CH_3NH_3^+$) or formamidinium ($NH_2CHNH_2^+$),** B is **a big inorganic cation - usually lead(II) (Pb^{2+}) and** X is **slightly smaller halogen anion – usually chloride (Cl^-) or iodide (I^-)** that bonds to both. Perovskite structures are made up of a variety of different elements. Scientists can design perovskite crystals with a wide range of physical, optical, and electrical properties using this compositional flexibility. Ultrasound machines, memory chips. But our main goal is the use of these kind of materials in solar cells.

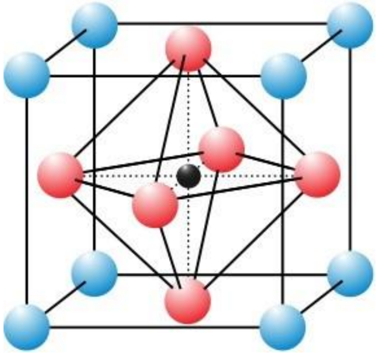


Figure 3.1.1 : A schematic of a perovskite crystal

Perovskite as Photovoltics

Synthetic perovskites are being recognized as potential inexpensive base materials for high-efficiency commercial photovoltaics, and solar cells are currently the most popular perovskite application. The bandgap of perovskite photovoltaics is very large. This offers the possibility of integrating them with low-bandgap photovoltaic technology, resulting in increased efficiency, which is significant in a highly competitive market where device costs are determined by efficiencies. Perovskite solar cells also have a range of advantages, including durability, semitransparency, thin-film, light weight, and low processing costs.

Synthetic perovskites have been described as potential low-cost base materials for high-performance commercial photovoltaics;[2] NREL announced a conversion efficiency of up to 25.5 percent in 2020,[2][3][4] and they can be made using the same thin-film manufacturing techniques as thin-film silicon solar cells.[5] In dye-sensitized solar cells, methylammonium tin halides and methylammonium lead halides are of concern.[6][7] A team of researchers led by Dr. Alexander Weber-Bargioni demonstrated in July 2016 that perovskite PV cells could theoretically achieve a peak efficiency of 31%.[8]

The methylammonium lead triiodide (CH 3NH 3PbI 3) is the most common of the methylammonium halides studied thus far. It has a high charge carrier mobility and lifespan, allowing light-generated electrons and holes to travel far enough to be removed as current rather than losing energy as heat inside the cell. Both electrons and holes have effective diffusion lengths of about 100 nm in CH 3NH 3PbI

3.2 Perovskite Solar Cells

Basic Structure

A perovskite solar cell uses a perovskite-structured compound as the light-harvesting active layer, most commonly a hybrid organic-inorganic lead or tin halide-based material. In 2013, a revolutionary PSC architecture called the inverted planar perovskite solar cell was developed. The bottom (HTL – hole transport material) and top (ETL– electron transport material) charge transport layers in this type of cell are p-type and n-type materials, respectively.

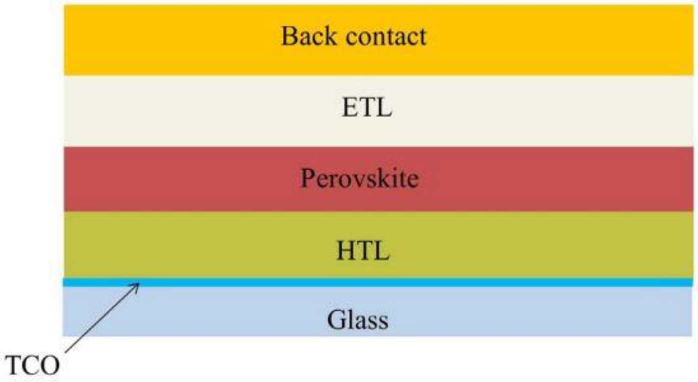


Figure 3.2.1: **Schematic image of an inverted planar perovskite solar cell**

Researchers have made efforts to improve the quality of perovskite semiconducting materials, resulting in an increase in low cost and high performance in solar cell capacitance simulator-one dimension simulation (SCAPS). In 2016, talks about the device simulation of lead-free CH3NH3SnI3perovskite solar cells with high efficiency. He discovered that by changing the doping concentration of the perovskite absorption layer and the electron affinity of the buffer and HTM during simulation, the solar cell efficiency can be improved to some degree, thus lowering the defect density of the perovskite absorption layer improves the cell performance significantly. They increased the PCE to 23.36 percent, the JSC to 31.59mA/cm2, the OC to 0.92V, and the FF to 79.99 percent by further optimizing. [10] In 2017, Seok and co-workers introduced an approach to reduce defects in the perovskite layer by using an intra-molecular exchanging technique, which is advantageous in reducing defect concentration, and they achieved an efficiency of over 22%. [11] In 2018, a Comparative Study of Different ETMs in Perovskite Solar Cells with Inorganic Copper Iodide as HTM was carried out, indicating Lead-based perovskite solar cells (CH3NH3PbI3 PSC) with CuI as HTM, TCO, IDL, and different ETMs (TiO2, CdS, ZnSe, ZnO, ZnOS) are studied by SCAPS Simulation, indicating CuI as the highest PCE achieved is 23.47%. The thickness of the layers has a significant impact on the solar cell's efficiency parameters. We get a PCE of 26.11 percent after optimizing the thickness of all the layers.

3.3 GENERAL MODEL

A simple model for a planar perovskite solar cell of n-i-p device structure consists of mainly five layers.

3.3.1 TCO

Doped metal oxides called transparent conductive oxides (TCO) are used in optoelectronic devices like flat panel displays and photovoltaics (including inorganic devices, organic devices, and dye-sensitized solar cells). Researchers have found that the layer on top of ETM can be mainly ITO (Indium Tin Oxide) and FTO (Fluorine doped Tin Oxide). ITO is generally more expensive than FTO. FTO has better transmission rate in visible wavelength.

3.3.2 ETL

The most important property of an ETL is that it must correspond with the perovskite layer in terms of lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO) above the perovskite active layer. It must have a high UV-Vis transmittance so that a photon can quickly pass through and be absorbed by the perovskite absorber. Exciton generation across the perovskite layer through light absorption must be dissociated before being collected by the ETL or HTL.

Metal oxides such as TiO2, ZnO, SnO2, SiO2, and ZrO2 can be used as ETL or scaffolding materials. Each material has its own set of benefits that help to increase PCE. PSC has been rendered using two different types of solution methods. The average PCE of rutile-perovskite solar cells was 8.19 percent, and the average PCE of anatase-perovskite solar cells was 7.23 percent. To monitor the shunt resistance and series resistance, researchers have predicted that an optimum porosity and an optimum over layer of perovskite are needed and successfully modified the particle size of rutile TiO_2 using chemical bath-deposited rutile thin films and $TiCl_4$ treatment at various concentrations.

- **METAL OXIDE AS ETL**

Miyasaka's group (Tokyo Univ.) formed the PSC in 2009. They successfully sensitized TiO_2 for visible-light conversion in photo electrochemical cells with photo voltage of 0.97 V and PCE of 3.8 percent using two different forms of organo-lead halide perovskite nanocrystals, $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$.

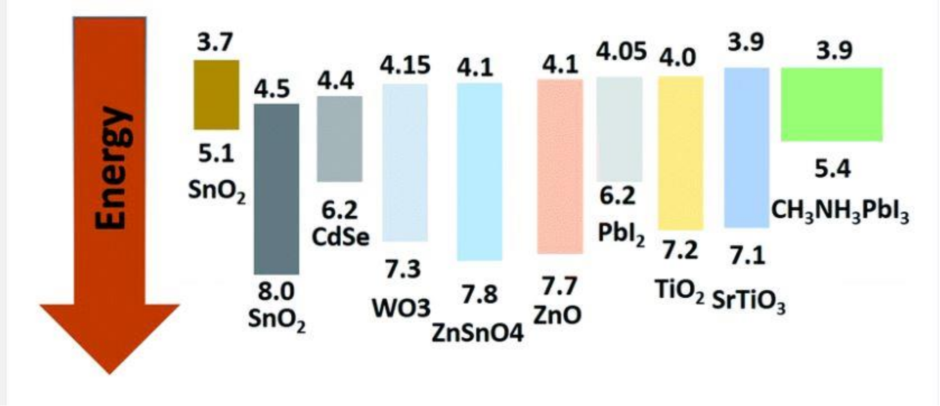


Figure 3.3 : ETL with respect to perovskite Band energy diagram of different.

Later study by Park's (Sungkyunkwan Univ.), Snaith's (Oxford Univ.), and Gratzel's (Ecole Polytechnique) groups greatly advanced PSC research and achieved efficiency of more than 15%. To control the environment, the PSC initially needed a glove box. Yang's (UCLA) research group recently posted a 19.3 percent efficiency rate.[16] Furthermore, tuning the band gap and Fermi level, which can increase or decrease the open circuit voltage, was shown to improve efficiency in doped ETM. The Fermi level can be raised using n-type doping in transition metal oxide ETM, allowing for a smooth electron injection from the perovskite active layer. Many groups have also used core–shell nanoparticles Al_2O_3/ZnO,[17] TiO_2/MgO,[18] and WO_3/TiO_2 [19] for charge retardation, and improved charge recombination resistance by insulating material with efficient charge injection and charge transport.

3.3.3 PEROVKSITE LAYER

The perovskite materials, out of all the components of perovskite solar cells, play a critical role in light absorption and photoelectric conversion. Single ions occupying each of the A-, B-, and X-sites in perovskite compositions. The optimization of materials and structures is one of the keys to improving the photoelectric conversion efficiency.

In recent years, researchers have focused on the more complex structures of mixed A- and X-site perovskites. Three of the NREL's six certified efficiencies is focused on the (FA/MA)Pb(I/Br) and (Cs/FA/MA)Pb(I/Br) perovskite schemes, as shown in Figure. When compared to FAPbI3-based perovskite solar cells, the (FA/MA)Pb(I/Br) system displayed improved stability under storage conditions in air (50 percent RH, 23°C) without encapsulation, according to Zheng et al.

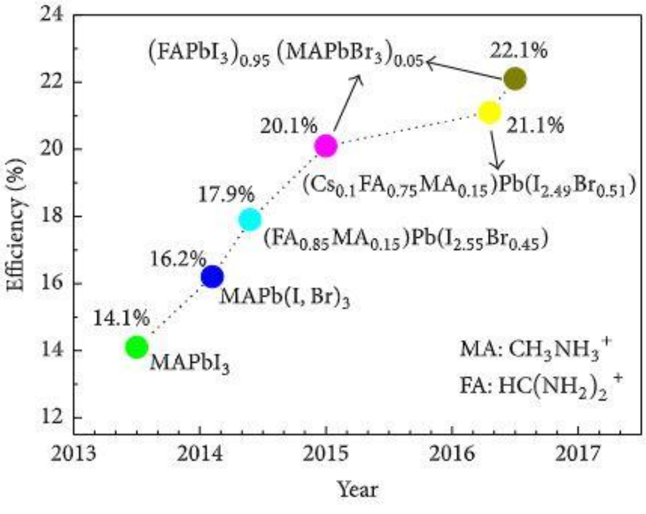


Figure 3.3.3 : The best efficiencies of perovskite solar cells certified by the NREL

As MABr is introduced into alloys with FAPbI3, the lattice size is minimized, and the strain forces are relaxed, according to the theory. The pseudocubic-phase is therefore preserved at room temperature and also in humid air in this manner. The research on (Cs/FA/MA)Pb(I/Br) and (Rb/Cs/FA/MA)Pb(I/Br) ternary and quaternary mixed cation systems primarily focused on the design of multicomponent perovskites to achieve a robust, single, pure step that can allow the construction of stable structures with optimal transport and even higher PCEs.

3.3.4 HTL

The ideal hole transport layer (HTL) will have a high hole mobility, close alignment with the perovskite valence band, strong conductivity, and higher stability. PSCs use organic, inorganic, and polymeric materials as the hole transport layer.

Inorganic hole transport materials are normally amorphous semiconductors The hole transport layer's primary function is to capture and transport holes from the perovskite light-absorbing layer in order to aid in the isolation of electron-hole pairs in perovskite materials by cooperating with the electron transport layer. For hole transport, the highest occupied molecular orbit (HOMO) in hole transport materials must fit the valence band of perovskite materials.

because the crystallization of the HTL can reduce the contact at the perovskite/HTL interface. After being deposited on the substrate, certain inorganic materials require sintering. Since perovskite can be degraded by high temperatures, some inorganic hole transfer materials can only be used in inverted configuration PSCs. Inorganic hole transfer materials have a greater stability than polymer/organic materials HTL, which is a benefit for PSCs. PSCs can use most inorganic hole transfer materials without doping.

3.4 PROPSED MODEL

Here inverted planar perovskite solar cell model is used to make it more efficient and reduce overall cost. By comparing two different ETL we are trying to find an optimum result. In one model we are using ZnO as ETL and in another we're using CdS as ETL.

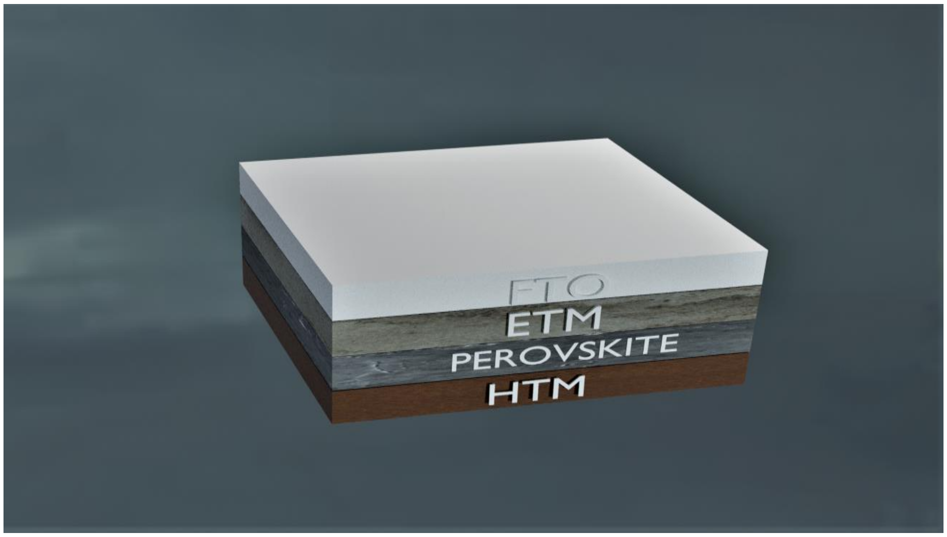


Figure 3.4.1 : 3D view of Perovskite model

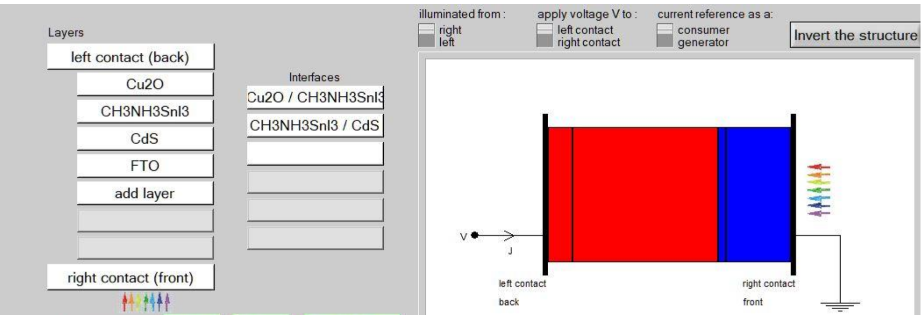


Figure 3.4.2 : Perovskite Model (CdS as ETL)

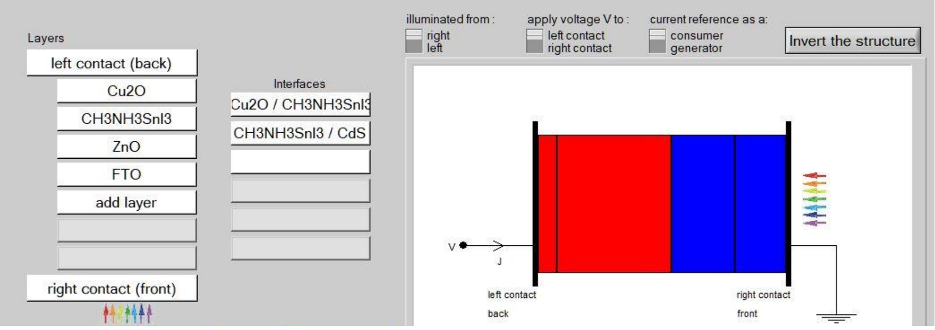


Figure3.4.3 : Perovskite model (ZnO as ETL)

CHAPTER 4

METHODOLOGY

4.1 SCAPS 1D

SCAPS (Solar Cell Capacitance Capacitor) is a software that simulates solar cells in one dimension. It was first created at the University of Gent's Department of Electronics and Information Systems (ELIS). This software is freely accessible to researchers all over the world and is growing in popularity as a simple but powerful solar cell analysis tool.

The software was created for CuInSe2 (Cu(In,Ga)Se2 and CdTe(CdS, ZnO, etc.) and CdTe(CdS, ZnO, etc.) cell structures. Recent advancements have made the software applicable to both crystalline and amorphous solar cells (Si and GaAs family) (a-Si and micromorphous Si). The key simulation has the following functions:

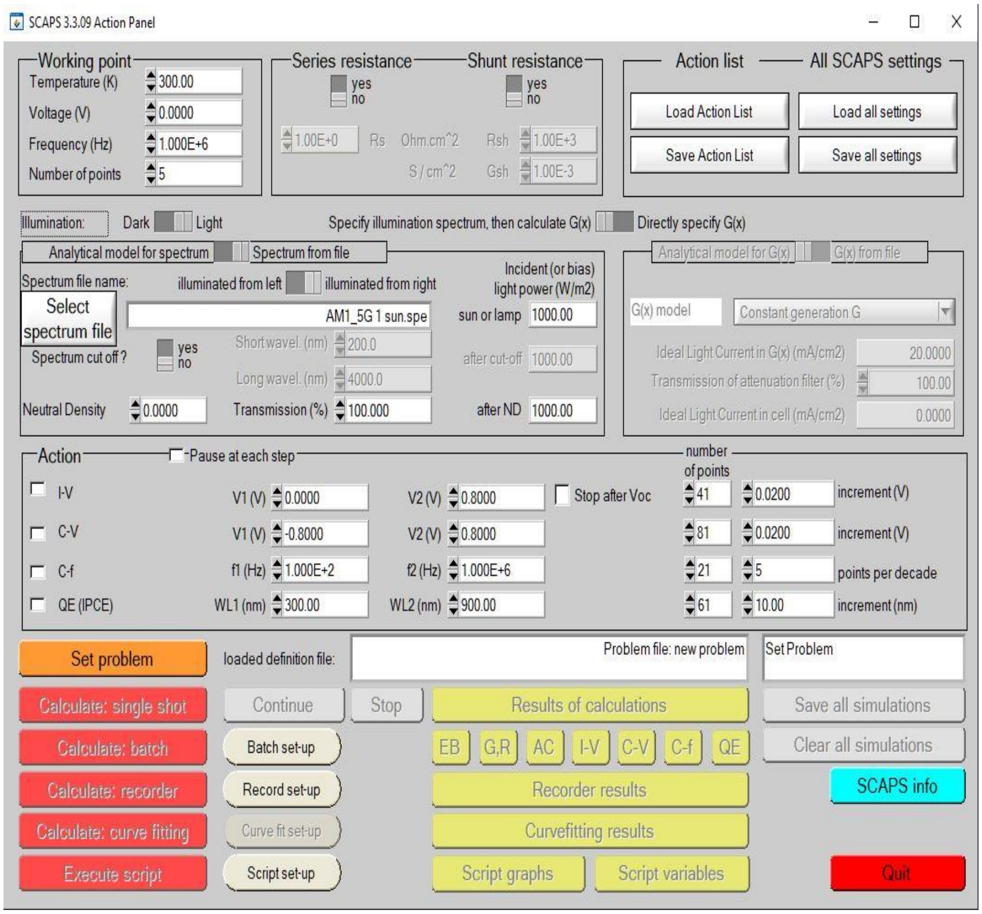
- Output for I/V, C/V, C/f, Q(l), band diagrams, concentrations, and currents
- Data analysis for I-V, C-V, C-f
- A number of standard models available with the distribution package
- User interface is well-designed, and scripting is easy.

Simulation Procedure:

This chapter is consisting of the work processes and methods used to build the desired model we are discussing for the whole book. The project was totally dependent on SCAPS-1D. As a result, the work process will be mostly as setting layers and values for material, defect, and interface parameters available in SCAPS.

4.1.1 ACTION PANEL

In the action panel, the illumination was tuned to dark to light and the spectrum file selected was AM1_5G sun.spe This AM1.5 Global spectrum is designed for flat plate modules and has an integrated power of 1000 W/m^2 (100 mW/cm^2) . Temperature, voltage, frequency, number of points were kept standard.



SCAPS 3.3.09 Action Panel

Working point

Temperature (K) 300.00

Voltage (V) 0.0000

Frequency (Hz) 1.000E+6

Number of points 5

Series resistance: yes / no — Rs 1.00E+0 Ohm.cm^2

Shunt resistance: yes / no — Rsh 1.00E+3 — Gsh 1.00E-3 S / cm^2

Illumination: Dark / Light

Specify illumination spectrum, then calculate G(x) / Directly specify G(x)

Analytical model for spectrum / Spectrum from file

Spectrum file name: illuminated from left / illuminated from right

AM1_5G 1 sun.spe

Incident (or bias) light power (W/m2)

sun or lamp 1000.00

after cut-off 1000.00

after ND 1000.00

Spectrum cut off ? yes / no

Short wavel. (nm) 200.0

Long wavel. (nm) 4000.0

Neutral Density 0.0000

Transmission (%) 100.000

Analytical model for G(x) / G(x) from file

G(x) model Constant generation G

Ideal Light Current in G(x) (mA/cm2) 20.0000

Transmission of attenuation filter (%) 100.00

Ideal Light Current in cell (mA/cm2) 0.0000

Action ☐ Pause at each step

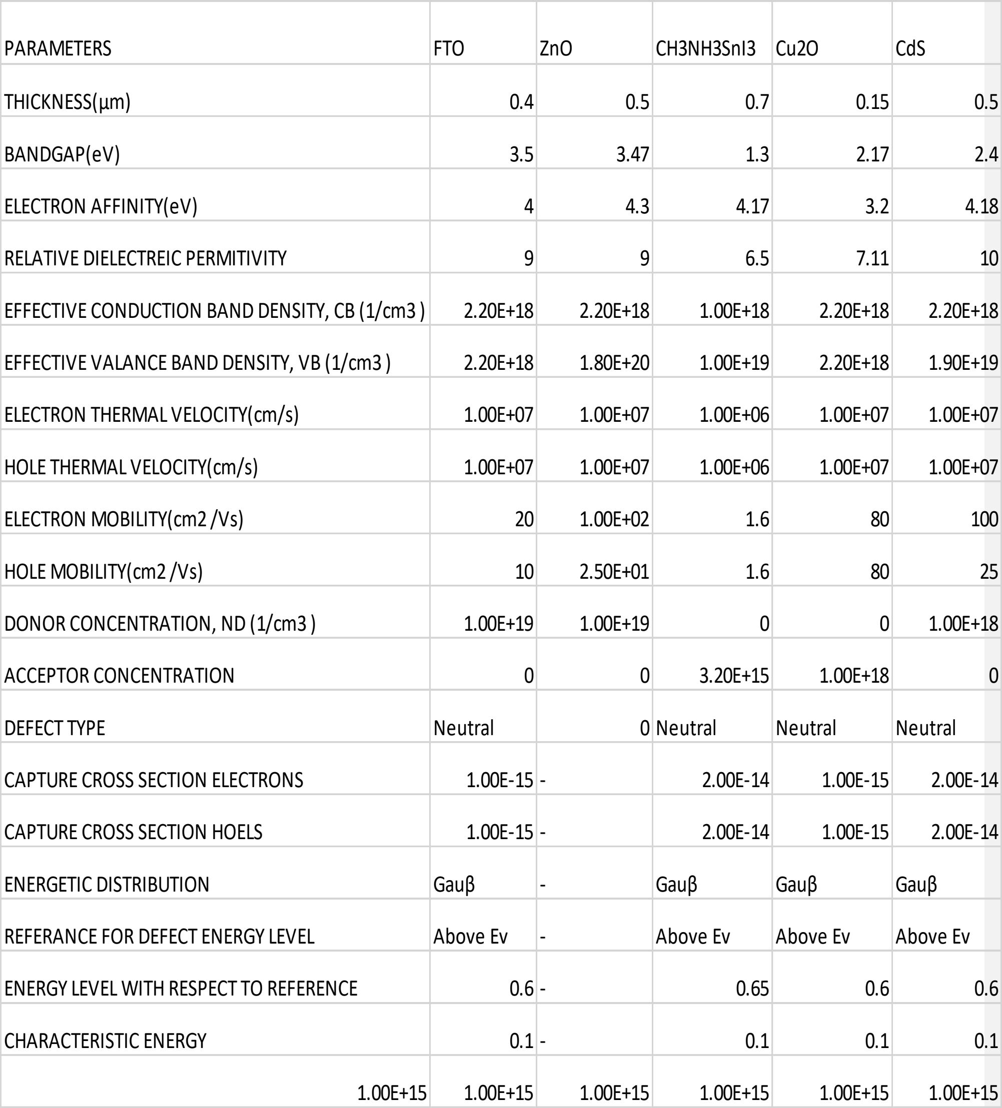
						number of points		
☐	I-V	V1 (V)	0.0000	V2 (V)	0.8000 ☐ Stop after Voc	41	0.0200	increment (V)
☐	C-V	V1 (V)	-0.8000	V2 (V)	0.8000	81	0.0200	increment (V)
☐	C-f	f1 (Hz)	1.000E+2	f2 (Hz)	1.000E+6	21	5	points per decade
☐	QE (IPCE)	WL1 (nm)	300.00	WL2 (nm)	900.00	61	10.00	increment (nm)

loaded definition file: Problem file: new problem

Set Problem

Figure 4.1.1 : Action Panel

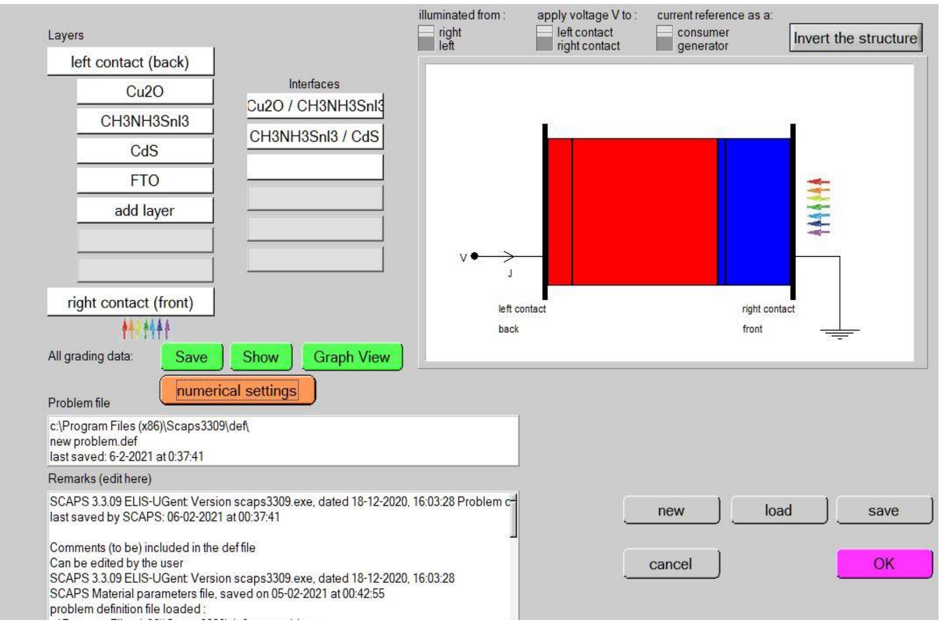
4.2 DATA TABLE



PARAMETERS	FTO	ZnO	CH3NH3SnI3	Cu2O	CdS
THICKNESS(µm)	0.4	0.5	0.7	0.15	0.5
BANDGAP(eV)	3.5	3.47	1.3	2.17	2.4
ELECTRON AFFINITY(eV)	4	4.3	4.17	3.2	4.18
RELATIVE DIELECTREIC PERMITIVITY	9	9	6.5	7.11	10
EFFECTIVE CONDUCTION BAND DENSITY, CB (1/cm3)	2.20E+18	2.20E+18	1.00E+18	2.20E+18	2.20E+18
EFFECTIVE VALANCE BAND DENSITY, VB (1/cm3)	2.20E+18	1.80E+20	1.00E+19	2.20E+18	1.90E+19
ELECTRON THERMAL VELOCITY(cm/s)	1.00E+07	1.00E+07	1.00E+06	1.00E+07	1.00E+07
HOLE THERMAL VELOCITY(cm/s)	1.00E+07	1.00E+07	1.00E+06	1.00E+07	1.00E+07
ELECTRON MOBILITY(cm2 /Vs)	20	1.00E+02	1.6	80	100
HOLE MOBILITY(cm2 /Vs)	10	2.50E+01	1.6	80	25
DONOR CONCENTRATION, ND (1/cm3)	1.00E+19	1.00E+19	0	0	1.00E+18
ACCEPTOR CONCENTRATION	0	0	3.20E+15	1.00E+18	0
DEFECT TYPE	Neutral	0	Neutral	Neutral	Neutral
CAPTURE CROSS SECTION ELECTRONS	1.00E-15	-	2.00E-14	1.00E-15	2.00E-14
CAPTURE CROSS SECTION HOELS	1.00E-15	-	2.00E-14	1.00E-15	2.00E-14
ENERGETIC DISTRIBUTION	Gauβ	-	Gauβ	Gauβ	Gauβ
REFERANCE FOR DEFECT ENERGY LEVEL	Above Ev	-	Above Ev	Above Ev	Above Ev
ENERGY LEVEL WITH RESPECT TO REFERENCE	0.6	-	0.65	0.6	0.6
CHARACTERISTIC ENERGY	0.1	-	0.1	0.1	0.1
1.00E+15	1.00E+15	1.00E+15	1.00E+15	1.00E+15	1.00E+15

4.3 Perovskite model (CdS as ETM)

- Setting the layers as following: Left Contact (back) - Cu2O (HTM) – CH3NHESNI3(Perovskite layer)- CdS (ETM) – FTO
- The structure is selected as non inverted.



Problem file

c:\Program Files (x86)\Scaps3309\def\
new problem.def
last saved: 6-2-2021 at 0:37:41

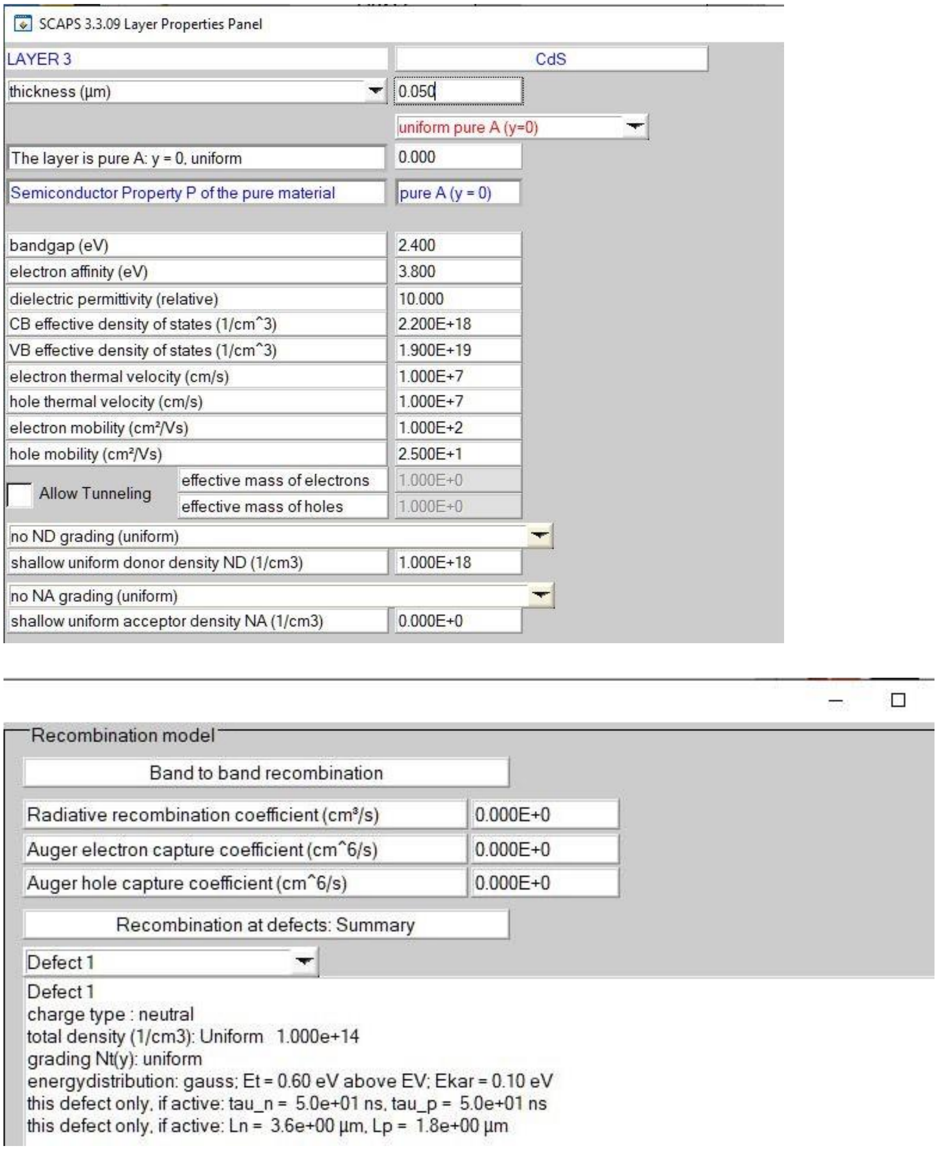
Remarks (edit here)

SCAPS 3.3.09 ELIS-UGent: Version scaps3309.exe, dated 18-12-2020, 16:03:28 Problem c
last saved by SCAPS: 06-02-2021 at 00:37:41

Comments (to be) included in the def file
Can be edited by the user
SCAPS 3.3.09 ELIS-UGent: Version scaps3309.exe, dated 18-12-2020, 16:03:28
SCAPS Material parameters file, saved on 05-02-2021 at 00:42:55
problem definition file loaded :

Figure 4.3.1: Perovskite layout for CdS as ETM

Then from data table 4.2 we need to set all the parameters.



SCAPS 3.3.09 Layer Properties Panel

LAYER 3	CdS
thickness (µm)	0.050
	uniform pure A (y=0)
The layer is pure A: y = 0, uniform	0.000
Semiconductor Property P of the pure material	pure A (y = 0)
bandgap (eV)	2.400
electron affinity (eV)	3.800
dielectric permittivity (relative)	10.000
CB effective density of states (1/cm^3)	2.200E+18
VB effective density of states (1/cm^3)	1.900E+19
electron thermal velocity (cm/s)	1.000E+7
hole thermal velocity (cm/s)	1.000E+7
electron mobility (cm²/Vs)	1.000E+2
hole mobility (cm²/Vs)	2.500E+1
☐ Allow Tunneling effective mass of electrons	1.000E+0
effective mass of holes	1.000E+0
no ND grading (uniform)	
shallow uniform donor density ND (1/cm3)	1.000E+18
no NA grading (uniform)	
shallow uniform acceptor density NA (1/cm3)	0.000E+0

Recombination model

Band to band recombination

Radiative recombination coefficient (cm³/s)	0.000E+0
Auger electron capture coefficient (cm^6/s)	0.000E+0
Auger hole capture coefficient (cm^6/s)	0.000E+0

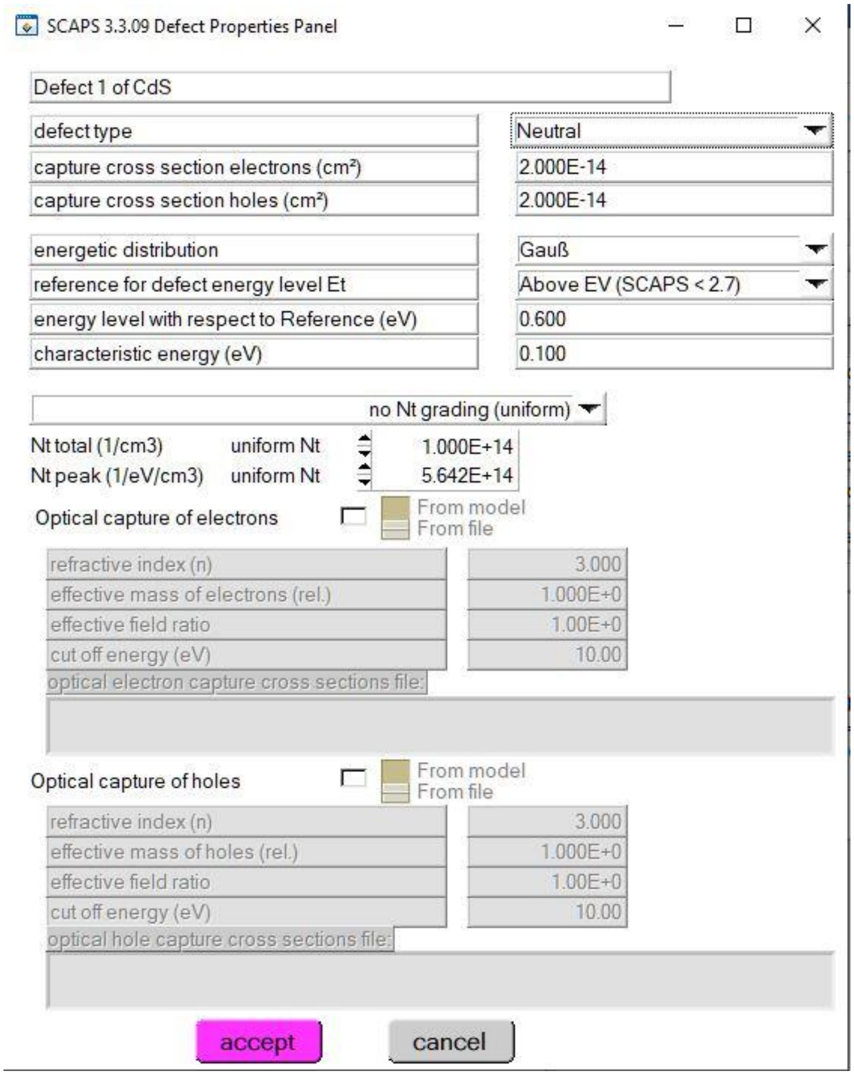
Recombination at defects: Summary

Defect 1

Defect 1
charge type : neutral
total density (1/cm3): Uniform 1.000e+14
grading Nt(y): uniform
energydistribution: gauss; Et = 0.60 eV above EV; Ekar = 0.10 eV
this defect only, if active: tau_n = 5.0e+01 ns, tau_p = 5.0e+01 ns
this defect only, if active: Ln = 3.6e+00 µm, Lp = 1.8e+00 µm

Fig 4.3.2 : Setting parameters

After that, set all the defect parameters.



SCAPS 3.3.09 Defect Properties Panel

Defect 1 of CdS

defect type	Neutral
capture cross section electrons (cm²)	2.000E-14
capture cross section holes (cm²)	2.000E-14
energetic distribution	Gauß
reference for defect energy level Et	Above EV (SCAPS < 2.7)
energy level with respect to Reference (eV)	0.600
characteristic energy (eV)	0.100

no Nt grading (uniform)

Nt total (1/cm3)	uniform Nt	1.000E+14
Nt peak (1/eV/cm3)	uniform Nt	5.642E+14

Optical capture of electrons ☐ From model / From file

refractive index (n)	3.000
effective mass of electrons (rel.)	1.000E+0
effective field ratio	1.00E+0
cut off energy (eV)	10.00

optical electron capture cross sections file:

Optical capture of holes ☐ From model / From file

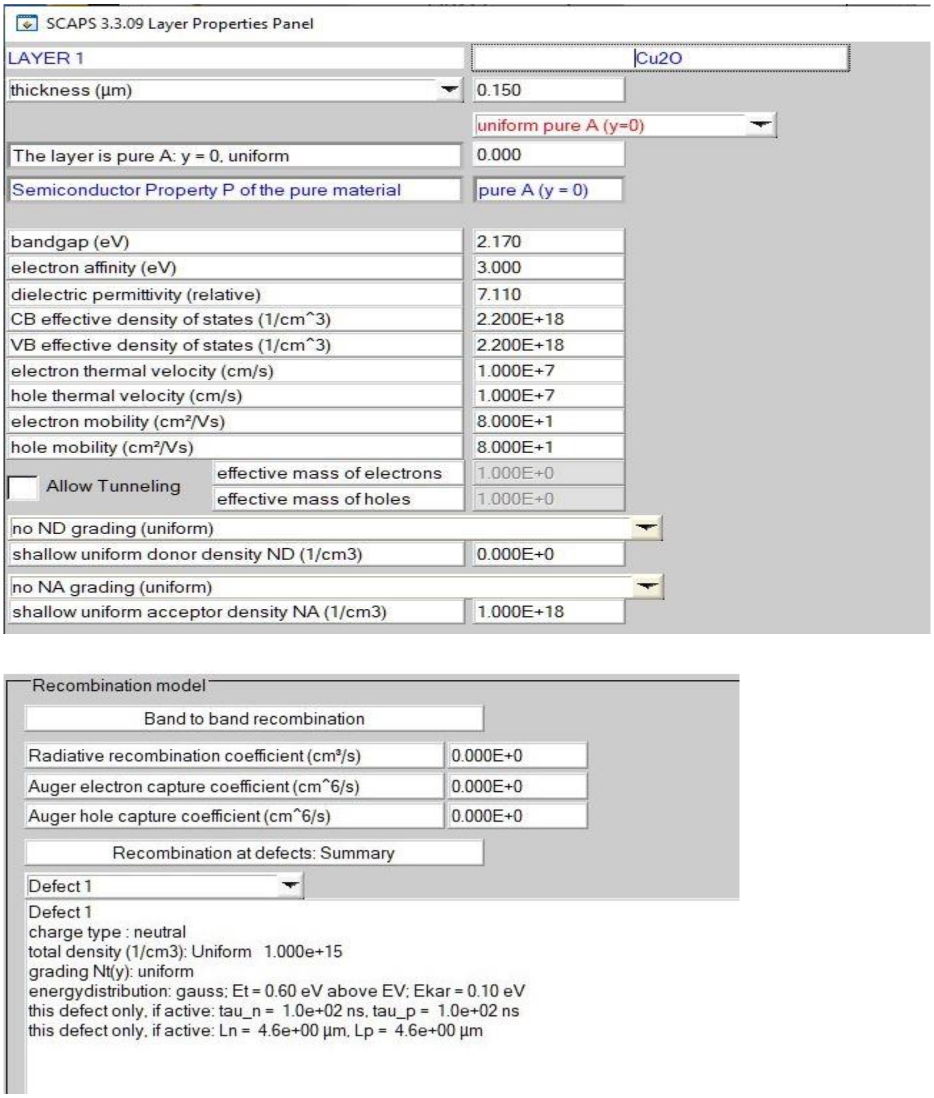
refractive index (n)	3.000
effective mass of holes (rel.)	1.000E+0
effective field ratio	1.00E+0
cut off energy (eV)	10.00

optical hole capture cross sections file:

Fig 4.3.3 : Setting defect parameters

- Setting interface parameters

1. Cu2O ad Perovskite Interface


SCAPS 3.3.09 Layer Properties Panel

LAYER 1	Cu2O
thickness (µm)	0.150
	uniform pure A (y=0)
The layer is pure A: y = 0, uniform	0.000
Semiconductor Property P of the pure material	pure A (y = 0)
bandgap (eV)	2.170
electron affinity (eV)	3.000
dielectric permittivity (relative)	7.110
CB effective density of states (1/cm^3)	2.200E+18
VB effective density of states (1/cm^3)	2.200E+18
electron thermal velocity (cm/s)	1.000E+7
hole thermal velocity (cm/s)	1.000E+7
electron mobility (cm²/Vs)	8.000E+1
hole mobility (cm²/Vs)	8.000E+1
☐ Allow Tunneling — effective mass of electrons	1.000E+0
effective mass of holes	1.000E+0
no ND grading (uniform)	
shallow uniform donor density ND (1/cm3)	0.000E+0
no NA grading (uniform)	
shallow uniform acceptor density NA (1/cm3)	1.000E+18

Recombination model

Band to band recombination

Radiative recombination coefficient (cm³/s)	0.000E+0
Auger electron capture coefficient (cm^6/s)	0.000E+0
Auger hole capture coefficient (cm^6/s)	0.000E+0

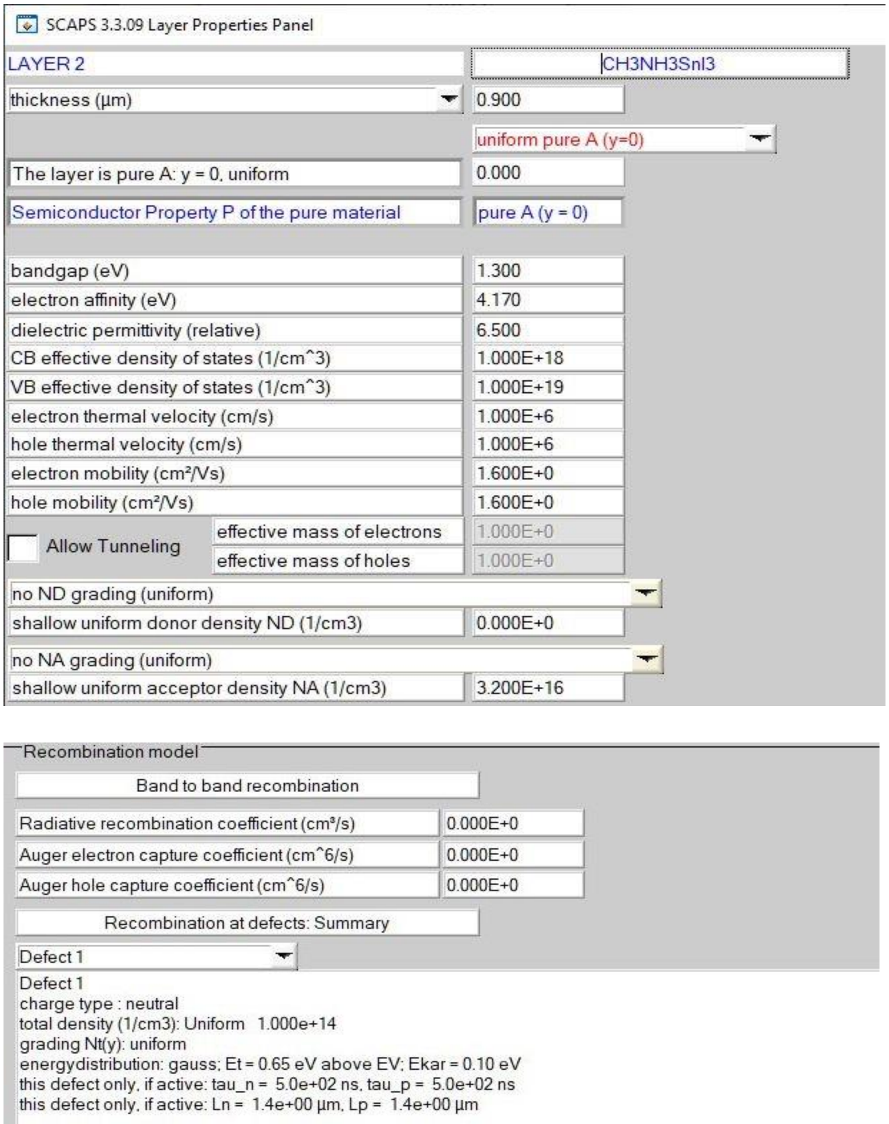
Recombination at defects: Summary

Defect 1

Defect 1
charge type : neutral
total density (1/cm3): Uniform 1.000e+15
grading Nt(y): uniform
energydistribution: gauss; Et = 0.60 eV above EV; Ekar = 0.10 eV
this defect only, if active: tau_n = 1.0e+02 ns, tau_p = 1.0e+02 ns
this defect only, if active: Ln = 4.6e+00 µm, Lp = 4.6e+00 µm

Fig 4.3.4 : Cu2O & Perovskite interface parameter

2. Perovskite & CdS parameters



LAYER 2: CH3NH3SnI3

thickness (µm): 0.900

uniform pure A (y=0)

The layer is pure A: y = 0, uniform: 0.000

Semiconductor Property P of the pure material: pure A (y = 0)

bandgap (eV)	1.300
electron affinity (eV)	4.170
dielectric permittivity (relative)	6.500
CB effective density of states (1/cm^3)	1.000E+18
VB effective density of states (1/cm^3)	1.000E+19
electron thermal velocity (cm/s)	1.000E+6
hole thermal velocity (cm/s)	1.000E+6
electron mobility (cm²/Vs)	1.600E+0
hole mobility (cm²/Vs)	1.600E+0

☐ Allow Tunneling

effective mass of electrons: 1.000E+0

effective mass of holes: 1.000E+0

no ND grading (uniform)

shallow uniform donor density ND (1/cm3): 0.000E+0

no NA grading (uniform)

shallow uniform acceptor density NA (1/cm3): 3.200E+16

Recombination model

Band to band recombination

Radiative recombination coefficient (cm³/s)	0.000E+0
Auger electron capture coefficient (cm^6/s)	0.000E+0
Auger hole capture coefficient (cm^6/s)	0.000E+0

Recombination at defects: Summary

Defect 1

Defect 1
charge type : neutral
total density (1/cm3): Uniform 1.000e+14
grading Nt(y): uniform
energydistribution: gauss; Et = 0.65 eV above EV; Ekar = 0.10 eV
this defect only, if active: tau_n = 5.0e+02 ns, tau_p = 5.0e+02 ns
this defect only, if active: Ln = 1.4e+00 µm, Lp = 1.4e+00 µm

Fig 4.3.5 : Perovskite & CdS interface parameters

- After setting all these parameters we need to select single shot in action o panel and Select I-V and QE from Action bar.
- Then we need to simulate and find the result.

4.4 Perovskite model (ZnO as ETM)

- Setting the layers as following: Left Contact (back) - Cu2O (HTM) – CH3NH3SNI3(Perovskite layer)- ZnO (ETM) – FTO
- The structure is selected as non-inverted.

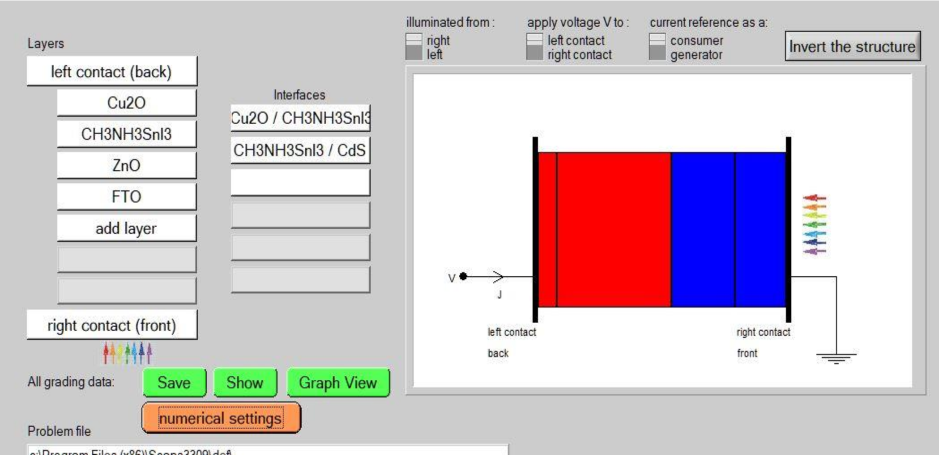


Figure 4.4 : Perovskite layout for ZnO as ETM

After this we need to repeat the same process from 4.3 and get results (I-V & QE) from simulation.

CHAPTER 5

RESULTS AND DISCUSSIONS

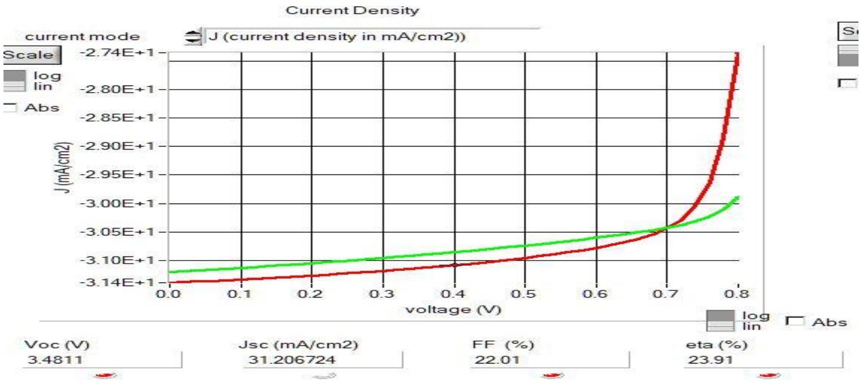
After setting up all parameters in both of the perovskite models, we get the analysis from each of the models. The two main characteristics we selected to be observed are I-V and QE. We also have 4 observations under I-V calculations which are -

Commented [SM1]:

- Voc (Open Circuit Voltage): The maximum amount of voltage that our models can provide under our defined conditions/parameters in an open circuit structure.
- Jsc (Short Circuit Current density): The maximum amount of current we can get from our cell in a given circuit.
- FF %(Fill Factor): Determines the maximum power from a solar cell.
- Eta %(Efficiency): The ratio between the output powers to the input power.

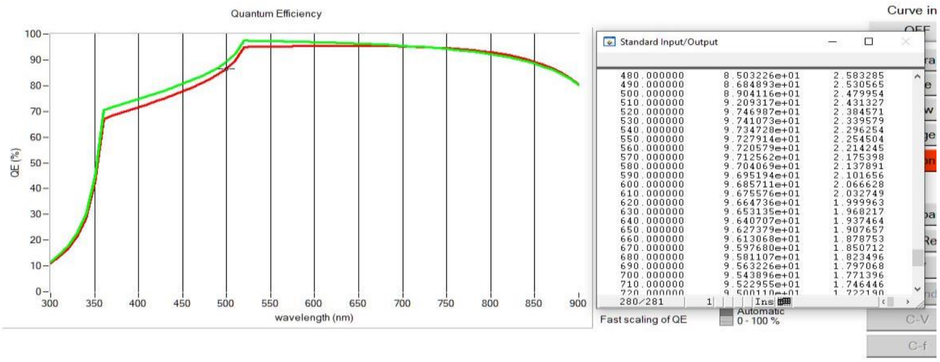
Finally, by QE we mean the ratio of the number of carriers collected by the solar cell to the number of photons of a given energy incident on the solar cell.

5.1 I-V and QE results of CdS model:



Voc (V) 3.4811
Jsc (mA/cm2) 31.206724
FF (%) 22.01
eta (%) 23.91

Fig 5.1.1: I-V curve and analysis of CdS as ETM



Standard Input/Output

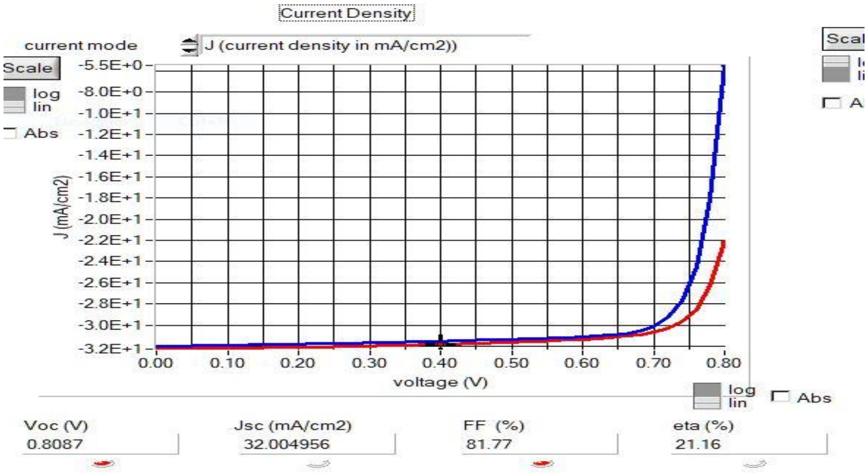
```
480.000000     8.503226e+01     2.583285
490.000000     8.684893e+01     2.530565
500.000000     8.904116e+01     2.479954
510.000000     9.209317e+01     2.431327
520.000000     9.746987e+01     2.384571
530.000000     9.741073e+01     2.339579
540.000000     9.734728e+01     2.296254
550.000000     9.727914e+01     2.254504
560.000000     9.720579e+01     2.214245
570.000000     9.712562e+01     2.175398
580.000000     9.704069e+01     2.137891
590.000000     9.695194e+01     2.101656
600.000000     9.685711e+01     2.066628
610.000000     9.675576e+01     2.032749
620.000000     9.664736e+01     1.999963
630.000000     9.653135e+01     1.968217
640.000000     9.640707e+01     1.937464
650.000000     9.627379e+01     1.907657
660.000000     9.613068e+01     1.878753
670.000000     9.597680e+01     1.850712
680.000000     9.581107e+01     1.823496
690.000000     9.563226e+01     1.797068
700.000000     9.543896e+01     1.771396
710.000000     9.522955e+01     1.746446
720.000000     9.500110e+01     1.722190
280/281     1     Ins
```

Fast scaling of QE: Automatic / 0 - 100 %

Fig 5.1.2 : QE curve and analysis of CdS as ETM

The highest value of **QE is 97.46%** which is in 520 nano meter.

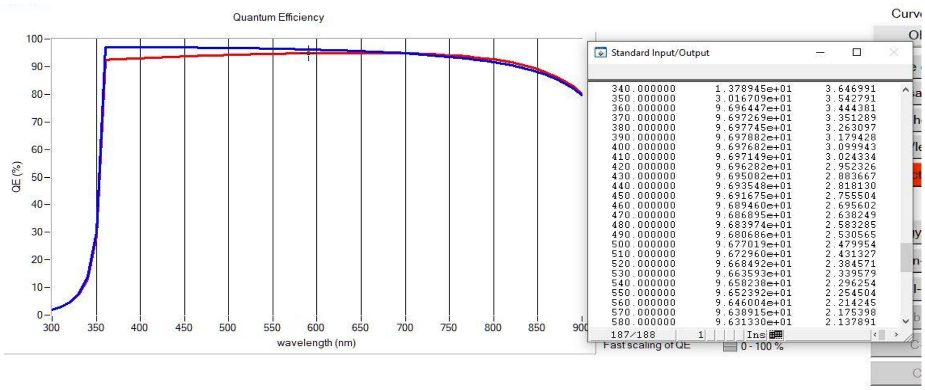
5.2 I-V and QE results of ZnO model:



current mode: J (current density in mA/cm2))

Voc (V): 0.8087
Jsc (mA/cm2): 32.004956
FF (%): 81.77
eta (%): 21.16

Fig 5.2.1 : I-V curve and analysis of ZnO as ETM



```
  340.000000      1.378945e+01      3.646991
  350.000000      3.016709e+01      3.542791
  360.000000      9.696447e+01      3.444381
  370.000000      9.697269e+01      3.351289
  380.000000      9.697745e+01      3.263097
  390.000000      9.697882e+01      3.179428
  400.000000      9.697682e+01      3.099943
  410.000000      9.697149e+01      3.024334
  420.000000      9.696282e+01      2.952326
  430.000000      9.695082e+01      2.883667
  440.000000      9.693548e+01      2.818130
  450.000000      9.691675e+01      2.755504
  460.000000      9.689460e+01      2.695602
  470.000000      9.686895e+01      2.638249
  480.000000      9.683974e+01      2.583285
  490.000000      9.680686e+01      2.530565
  500.000000      9.677019e+01      2.479954
  510.000000      9.672960e+01      2.431327
  520.000000      9.668492e+01      2.384571
  530.000000      9.663593e+01      2.339579
  540.000000      9.658238e+01      2.296254
  550.000000      9.652392e+01      2.254504
  560.000000      9.646004e+01      2.214245
  570.000000      9.638915e+01      2.175398
  580.000000      9.631330e+01      2.137891
```

Fig 5.2.2: QE curve and analysis of ZnO as ETM

The highest value of **QE is 96.978%** which is in 390 nano meter.

5.3 Comparing results

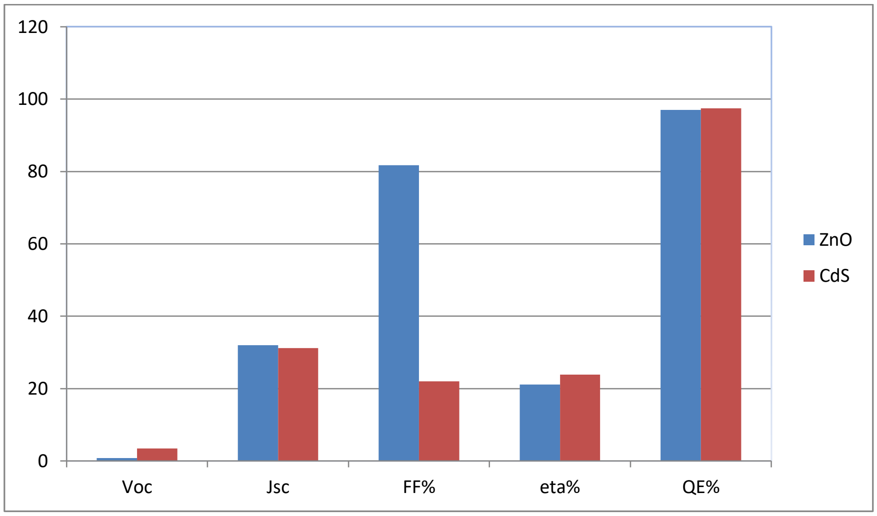
The values we get from the simulation keeping the TCO,HTM,Perovskite layer and both contacts constant and optimized-

Parameters	**ZnO as ETM**	**CdS as ETM**
Voc	0.8087	3.4811
Jsc	32.005	31.21
FF%	81.77	22.01

eta%	21.16	23.91
QE%	96.98	97.46

Table: I-V and QE values of proposed models

If we graph them out we get,



So, from the simulation, table and graph we can compare that,

- Open circuit voltage is much higher in CdS so can be used to operate high voltage equipment.
- Short circuit current density is almost same (31.206≈32.005) meaning both the models will provide same current in a given load.

- Quantum efficiency is almost same but in case of ZnO we get higher efficiency in a wider range (390nm~800nm) whereas CdS has less quantum efficiency range (520nm~800nm). That means ZnO can convert energy from lower wavelength light.
- Fill Factor is very high in ZnO.
- Conversion efficiency is a bit higher in CdS but by not a promising figure (0.5%)

But ZnO has lower market price and production cost than CdS(almost two to three times). Moreover ZnO is more ecofriendly or we can say that its recycling process is much easier and cheaper.

CHAPTER 6

CONCLUSION

Perovskite single junction solar cells can easily reach higher efficiency than most other solid state solar cells. So using perovskite materials and optimizing the other layers accordingly can bring about a revolutionary change in renewable energy sector.

Here we designed, optimized and simulated two Perovskite PV models considering the environmental effects, cost and efficiency. The optimization has been done based on previous researches, lab data and ideal data. We've taken two best candidates as perovskite material (CH3NH3SNI3) and HTM (Cu2O) and varied ETM(CdS & ZnO) layer.

From simulations and graphs we can conclude that CdS is slightly better than ZnO considering conversion efficiency and has an advantage in creating more voltage, whereas ZnO has more quantum efficiency.

However, the era of ever expanding civilization is largely dependent on advancement of technology- an advancing tool that is prominently influenced by industry, economics and interaction with nature. Keeping all these factors of influence and co dependence along with some other factors in mind, we find that ZnO is a more appealing candidate.

FUTURE WORKS

We have some potential targets that we want to accomplish based on the current state of our work.

- The optimization of different parameters of ZnO as ETM.
- Comparison of different HTM layers in perovskite solar cells.
- Optimization and co relation of different optimized ETM and HTM layers.
- Comparison between different types of defect in these layers.

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