ABOUT THE WORK AND OBJECTIVE

A conventional organic solar cell consists of a plastic or glass substrate material coated with a conducting layer of Indium Tin Oxide (ITO). There is a layer of donor-acceptor material on the substrate, which serves as active layer. The donor materials are small organic semiconducting materials, synthesized as discrete molecules with well-defined structures. These materials include pentacene, perylene dimides and fullerene derivatives. Fullerene and its derivatives are used as acceptors. Non-fullerene materials have also gained interest, of late. The donor and acceptor materials still have certain limitations that need to be addressed. These have been already mentioned above (limited absorption range, low carrier mobility, energy losses and recombination, low stability and degradation).

An attempt has been made in this work to address some pertinent issues. Instead of glass or plastic substrate, a bio degradable cellulose substrate has been used. The cellulose has been extracted from agricultural waste, which is generally discarded or burnt, thus giving it another potential use.

The active material is TiO2, which is an efficient material for the purpose. It has good thermal stability and can be easily synthesized as well as coated on the substrate material, unlike the donor-acceptor materials used in conventional organic solar cells. A dye has to be used with this active material to harvest the light and create the exciton pair needed for conduction. These dyes are quite expensive and have a short absorption range. The current work envisages and attempts to use the naturally occurring Light Harvesting Complexes (LHC's) from plant leaf extracts, instead of dyes.

Light harvesting complexes (LHCs) are assemblies of molecules that play a crucial role in capturing and transferring energy from sunlight in photosynthetic organisms. These complexes are responsible for absorbing light and directing the energy to reaction centres where it is utilized for photosynthesis (Scholes et al., 2011). LHCs are found in various photosynthetic systems, including plants, algae and bacteria. They consist of pigments, such as chlorophylls and carotenoids, which are responsible for absorbing light at different wavelengths. The absorbed light energy is then transferred through a process called energy transfer or resonance energy transfer, from one pigment molecule to another until it reaches the reaction centre. Whereas the dye is a pigment, the light harvesting complexes contain a series of sub protein molecules each possessing different valence and conduction bands.

One of the major reasons that have been understood from past studies and literature review for the fall of efficiency is the recombination effect. Recombination is an effect where the excited electron in the conduction band of the photoelectric active material, instead of getting collected at the ITO or FTO electrode, goes back to its own valance band.

LHCs are multi component in their constitution, with various protein molecules as the units. This gives them a wider range of absorption as well. Their incorporation in the system is expected to provide a number of levels in the matrix. These levels have been also supported by the UV-Vis analysis in the study.

It has been proposed in this work that due to the presence of multiple energy bands in the LHCs, the excited electron, instead of directly recombining to valance band of TiO2, goes to these intermediate levels of LHCs, thus providing an alternative path way to the electron to reach the electrode. This decreases the probability of recombination.

Polymers viz. Polypyrrole and Polyaniline have been used as counter electrodes. The interaction of functional groups in these polymers and the LHCs, called moieties, can also affect the performance of the device. This has been discussed in the thesis.

Solar Cells

1. SOLAR CELLS

Solar cells, also known as photovoltaic cells, are devices that convert sunlight directly into electricity. They are a vital component of the renewable energy harvesting techniques. Solar cells have undergone development through several generations of technological advancements, each characterized by improvements in efficiency, cost-effectiveness and manufacturing techniques. The various generations of solar cells are briefly given as under.

1.1. First Generation Solar Cells:

First-generation solar cells, also referred to as crystalline silicon (c-Si) solar cells, were developed in the 1950s and remain the most widely used solar cell technology today. (Docampo et al., 2013; Patidar et al., 2020). They are primarily made of silicon, a semiconductor material that has excellent properties for converting sunlight into electricity. Crystalline silicon cells can be further classified into two types: monocrystalline silicon (mono-Si) and polycrystalline silicon (poly-Si) (Tang et al., 2017).

Monocrystalline silicon solar cells are made from a single, continuous crystal structure, resulting in high efficiency and uniform appearance (Gu et al., 2023). They are produced by growing a large silicon crystal, which is then sliced into thin wafers. Monocrystalline cells typically have a higher cost due to the complex manufacturing process (Chahmi et al., 2023). Polycrystalline silicon solar cells, on the other hand, are made from multiple silicon crystals. The manufacturing process involves pouring molten silicon into a mold and allowing it to solidify, resulting in a less uniform appearance (Baby et al., 2022). Polycrystalline cells are less expensive to produce but generally have slightly lower efficiency compared to monocrystalline cells (Ullah & Rasul, 2018).

1.2. Second Generation Solar Cells:

Second-generation solar cells, also known as thin-film solar cells, emerged in the 1980s as an alternative to crystalline silicon cells. These cells are made by depositing thin layers of semiconductor materials onto a substrate, which can be glass, metal or plastic. Thin-film solar cells are much thinner and lighter than crystalline silicon cells and can be flexible, allowing for a wider range of applications.

There are several types of second-generation solar cells, including:

1.2.1. Cadmium Telluride (CdTe) Solar Cells:

CdTe solar cells are made by depositing a thin layer of Cadmium Telluride onto a substrate. CdTe solar cells are cost-effective to produce and have achieved high conversion efficiencies, making them commercially viable (Kim et al., 2019).

1.2.2. Copper Indium Gallium Selenide (CIGS) Solar Cells:

CIGS solar cells are made by depositing a thin layer of copper, indium, gallium, and selenium onto a substrate. CIGS cells have the potential for high efficiency and can be manufactured using low-cost processes, such as roll-to-roll printing (Islam et al., 2016).

1.2.3. Amorphous Silicon (a-Si) Solar Cells:

Amorphous silicon solar cells are made by depositing a non-crystalline form of silicon onto a substrate. Amorphous silicon cells have the advantage of being highly flexible and can be integrated into various materials, such as building materials and fabrics (Ma et al., 2014). However, they generally have lower efficiency compared to other thin-film technologies (Hwang et al. 2015).

1.3. Third Generation Solar Cells:

Third-generation solar cells are a category of emerging technologies that aim to overcome the limitations of previous generations. These technologies include a variety of approaches and materials, each with their own unique characteristics and potential advantages. While some third-generation solar cells are still in the research and development stage, others have begun to enter the commercial market (Dai et al., 2021, Lee et al., 2014). Here are a few examples:

1.3.1. Organic Solar Cells:

Organic solar cells, also known as organic photovoltaics (OPVs), utilize organic materials, typically carbon-based polymers or small molecules, as the active layer to absorb sunlight and generate electric current. Organic solar cells offer the advantage of being lightweight, flexible, and potentially low-cost to manufacture. They can be produced using solution-based processes such as printing or coating (Liang et al. (2010) Mrinalini et al., 2018; Tamai, 2020). However, their efficiency levels are still lower compared to traditional silicon-based cells, and they can be more susceptible to degradation over time.

Newer approaches and modifications in the development of organic solar cells are still evolving. This work is an attempt in the same direction.

1.3.2. Dye-Sensitized Solar Cells (DSSCs):

Dye-sensitized solar cells (DSSCs) use a photoelectrochemical system in which a photosensitive dye absorbs light and transfers electrons to a semiconductor material to generate an electric current. DSSCs can be manufactured using low-cost materials and processes and they have the benefit of working well under low-light conditions and indirect sunlight (Zhou et al. 2022). However, they have relatively lower conversion efficiencies compared to silicon-based cells (Ginting et al. 2017).

1.3.3. Perovskite Solar Cells:

Perovskite solar cells are a promising and rapidly advancing technology. They use a perovskite material, typically a hybrid organic-inorganic Lead Halide, as the light-absorbing layer. Perovskite solar cells have achieved high power conversion efficiencies comparable to silicon cells while being relatively simple and low-cost to manufacture (Yu et al. 2013). They can be fabricated using solution-based methods, such as spin-coating or inkjet printing (Pourjafari et al., 2022). However, perovskite cells face challenges related to stability and durability, as the material is sensitive to moisture and heat (Liu, 2023).

1.3.4. Quantum Dot Solar Cells:

Quantum dot solar cells utilize semiconductor nano crystals called quantum dots to absorb and convert sunlight into electricity (Dabbousi et al. 1997). Quantum dots can be engineered to absorb specific wavelengths of light by varying their size, allowing for tunability in the absorption spectrum (Uddin & Ghann 2018). This technology has the potential for high efficiency and can be processed using solution-based techniques (Bao & Bawendi 2015). However, quantum dot solar cells are still in the early stages of development, and further research is needed to improve their performance and stability.

1.4. Fourth Generation Solar Cells:

Fourth-generation solar cells are a conceptual category of advanced solar cell technologies that are still in the early stages of research and development. These technologies aim to overcome the limitations of previous generations and achieve even higher efficiencies and lower costs. Some of the approaches being explored in this generation include:

1.4.1. Multi-Junction Solar Cells:

Multi-junction solar cells consist of multiple semiconductor layers with different bandgaps stacked on top of each other. Each layer absorbs a specific wavelength of light, allowing for more efficient utilization of the solar spectrum (Feurer et al. 2018). Multi-junction cells have achieved impressive efficiency levels in specialized applications, such as space exploration and concentrated photovoltaics (Yamaguchi et al. 2021, Araki et al. 2019). However, their high cost and complexity limit their widespread use in terrestrial applications (Kang et al. 2016, Guo et al. 2022).

1.4.2. Tandem Solar Cells:

Tandem solar cells combine different types of solar cells, such as silicon and perovskite cells, in a stacked configuration. Each cell absorbs a specific portion of the solar spectrum, allowing for increased overall efficiency. Tandem cells have the potential to achieve high efficiencies while leveraging the advantages of different materials (Essig et al. 2015, Feurer et al., 2018, Guo et al., 2022). However, the challenge lies in developing efficient and stable interfaces between the different cell layers and managing the complex fabrication processes.

1.4.3. Nanostructured Solar Cells:

Nanostructured solar cells utilize materials with engineered nanostructures to enhance light absorption and charge carrier generation. These structures can include nano wires, nano tubes, or nano patterned surfaces that can trap and guide light within the cell, increasing the absorption path length (Lu & Lal 2010). Nanostructured solar cells have the potential to improve efficiency by maximizing light absorption and minimizing carrier recombination (Sun et al. 2020). However, their practical implementation and scalability remain areas of active research (Lee et al. 2014).

1.4.4. Integrated Solar Cells:

Integrated solar cells aim to integrate solar energy harvesting capabilities into various surfaces and objects, enabling seamless integration into everyday life. This includes solar cells integrated into windows, roofs, vehicles, and even clothing. The goal is to make solar energy generation ubiquitous and unobtrusive. Various technologies, such as transparent solar cells and flexible modules are being developed to enable this integration.

It is important to note that while these fourth-generation technologies hold great promise, they are still in the research and development phase. It takes time for new technologies to mature and become commercially viable. Additionally, the transition from one generation to another is not strictly defined, and there can be overlap between different generations as advancements continue to evolve.

Solar cells have evolved through different generations of technology, each with its own advancements and characteristics. From the first-generation crystalline silicon cells to the second-generation thin-film technologies and now the emerging third and fourth-generation approaches, solar cell technology has progressed in terms of efficiency, cost-effectiveness and versatility. Continued research and development in solar cell technology are essential to further improve efficiency, enhance stability, reduce costs and expand the range of applications, ultimately driving the growth of renewable energy and contributing to a sustainable future.

Cellulose

Use of Cellulose isolated from agricultural residues and other sources

Need and Rationale

India is an agricultural country and tons of agricultural residues are generated every year. They are used as fodder for cattle as well as in textile industries and other application. Tons of these residues still remain unutilized and are simply burnt off in some parts of the country causing enormous pollution (Jain et al. 2014, Jethva et al., 2019). These agricultural residues contain an extremely important material cellulose, which has great utility. The cellulose can be isolated and can be processed into sheets (Porichha et al., 2021). These sheets have good mechanical strength, extremely good flexibility, reasonably good thermal stability and very good transparency. These properties make use of cellulose films to be promising in several applications.

REPORT OF CROP PRODUCTION

According to the Indian Ministry of New and Renewable Energy (MNRE), India generates on an average 500 Million tons (Mt here after) of crop residue per year. The same report shows that a good amount of these crop residues are used as fodder and fuel for domestic as well as industrial purposes. However, there is still a surplus of 140 Mt out of which 92 Mt is burned each year. Table compares the agricultural waste generated by selected Asian countries in Mt/year. It is also interesting to note that the portion burnt as agricultural waste in India, in volume is much larger than the entire production of agricultural waste in other countries in the region.

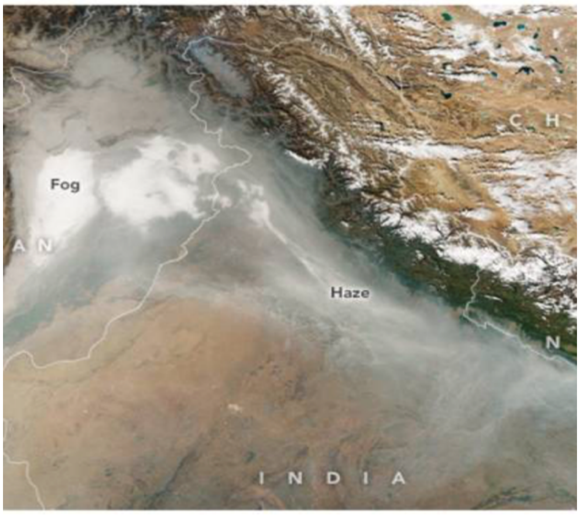

Figure 1: Burning of Agricultural Residues in India

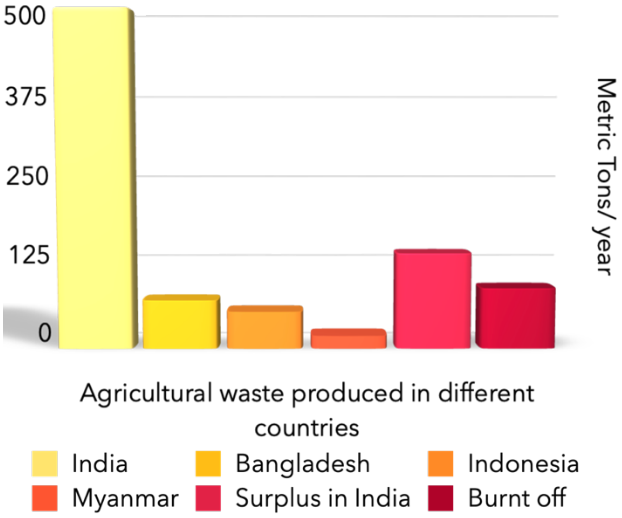

Figure 2: Pollution caused due to burning of agricultural remnants

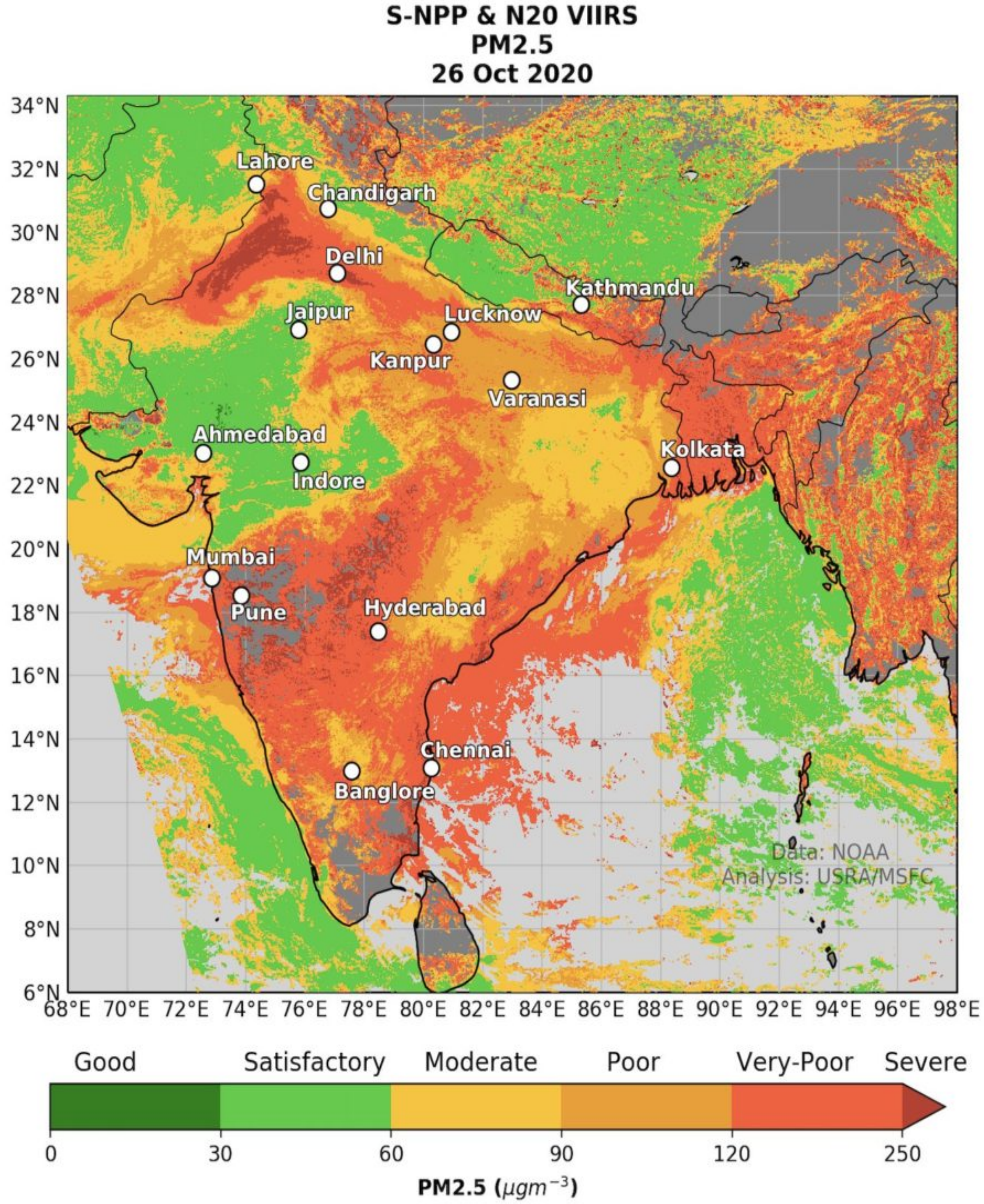

Figure 3: Thermal Image of Air Quality, rise in temperature and pollution caused due to burning of agricultural residues (Source of Image: Indian Ministry of New and Renewable Energy, MNRE)

The temperature varies from dark green to dark red in the ascending order

Cellulose is a naturally occurring polymer that is found abundantly in the plant cell wall. It is a major component of the plant cell wall, providing mechanical strength and rigidity to the plant cells. Cellulose is a linear polymer composed of glucose units linked by β-1,4-glycosidic bonds. It is the most abundant polysaccharide on earth and it is estimated that the annual production of cellulose by plants is around 180 billion tons.

Apart from cellulose, the plant cell wall also contains other components such as hemicelluloses, pectin, lignin, and proteins, which provide additional structural support to the plant cells and are essential for their growth and development.

Agricultural residues such as straw, corn stover, sugarcane bagasse and wood chips are rich sources of cellulose. These residues are generated in large quantities every year and their utilization can provide a sustainable source of cellulose for various industrial applications.

The structure of cellulose is highly ordered and crystalline, which gives it its unique properties such as high tensile strength, high surface area and excellent chemical stability. The cellulose molecule is composed of repeating units of glucose, which are arranged in a linear chain. The glucose units are linked by β-1,4-glycosidic bonds, which form long linear chains that are held together by hydrogen bonds.

One of the most promising applications of cellulose is in the production of transparent sheets for substrates for solar cells and other optoelectronic devices (Hou et al. 2020, Aburabie & Hashaikeh 2022). The high surface area due to the fibrous nature and cross linking as well as the high chemical stability of cellulose makes it an ideal material for use in these applications. In addition, cellulose is biodegradable and renewable, making it an environmentally friendly alternative (Nogi & Yano 2009).

In addition to its use in optoelectronic devices, cellulose has a wide range of applications in various industries. Cellulose is used in the production of paper and cardboard, textiles and food products such as ice cream, yogurt and processed meats (Balakrishnan et al. 2019). It is also used in the production of bio-fuels, as well as in the pharmaceutical and cosmetics industries.

The properties of cellulose can be modified through chemical and physical treatments, which can improve its performance and expand its range of applications (Wang et al. 2011). Cellulose can be chemically modified to make it more water-soluble, rendering it useful for the production of films and coatings. Physical treatments such as mechanical milling can be used to reduce the particle size of cellulose, which can improve its dispersibility and enhance its mechanical strength.

Despite the many advantages of cellulose, there are also some challenges associated with its use (Ma et al. 2019). One of the main challenges is the high energy and resource requirements for its extraction and processing. Another challenge is the difficulty in breaking down cellulose into its constituent glucose units, which limits its use as a feedstock for bio-fuels. However, advances in biotechnology and nanotechnology are providing new opportunities for the efficient and sustainable utilization of cellulose (Yin et al. 2020).

Recent developments in cellulose research have focused on the use of nanocellulose, which is produced by breaking down cellulose fibers into nanometer-sized particles (Wang et al. 2023). Nanocellulose has unique properties such as high tensile strength, high surface area and biocompatibility, which make it a promising material for various applications such as nanocomposites, biomedical devices and water purification (Nogi et al. 2015).

Another promising area of research is the use of cellulose-based materials as scaffolds for tissue engineering. Cellulose-based scaffolds can provide a three-dimensional structure for the growth of cells and tissues and they can be designed to mimic the properties of natural tissues such as cartilage and bone (Park et al. 2018). This approach has the potential to revolutionize the field of regenerative medicine, enabling the development of new treatments for a wide range of diseases and injuries.

In addition to its use in industrial and medical applications, cellulose also plays an important role in the global carbon cycle (Zhao et al. 2020). Plants use carbon dioxide from the atmosphere to produce cellulose through photosynthesis, which helps to regulate the levels of carbon dioxide in the atmosphere.

One of the major challenges in utilizing cellulose is its recalcitrance, which refers to its resistance to chemical and enzymatic degradation (Yang & Berglund 2020). This makes it difficult to extract glucose from cellulose, particularly for bio-fuel production. To address this challenge, researchers are exploring new methods for breaking down cellulose, such as the use of ionic liquids or genetically engineered enzymes.

Another area of research is the development of cellulose-based materials with enhanced properties, such as improved mechanical strength, water resistance, and biodegradability. This can be achieved through the incorporation of other natural polymers, such as chitin or lignin, or through the use of chemical and physical treatments to modify the properties of cellulose (Labidi et al. 2019).

Finally, the sustainable production and utilization of cellulose is an important area of research, as it has the potential to reduce the environmental impact of various industries. This can be achieved through the development of more efficient methods for cellulose extraction and processing, as well as the use of agricultural and forestry residues as feed-stocks for cellulose production.

SOURCES OF CELLULOSE

Cellulose is one of the most abundant organic compounds on earth. It is a complex polysaccharide that forms the structural component of the cell walls of plants, algae and some bacteria. The molecule is composed of glucose units linked together by β-1,4-glycosidic bonds, forming long chains that are arranged in a crystalline structure. Cellulose is insoluble in water, but it is an important source of dietary fiber and is used in many industrial applications. In this section, the sources of cellulose are discussed in more detail.

1. Wood

One of the primary sources of cellulose is wood. Trees are composed of a combination of cellulose, hemi-cellulose and lignin. Cellulose is the primary component of the cell walls of wood fibers and it accounts for 40-50% of the dry weight of wood (Iwamoto et al. 2011). Wood is a renewable resource and is used in many industrial applications, including paper production, textile manufacturing and the production of bio fuels.

2. Cotton

Cotton is another significant source of cellulose. Cotton fibers are composed of nearly pure cellulose, with small amounts of other components like pectin, hemi-cellulose and lignin. Cotton is one of the most important agricultural crops in the world, and it is used extensively in the textile industry (Olsén et al. 2019).

3. Bamboo

Bamboo is a fast-growing, renewable source of cellulose. The stems of bamboo are composed of up to 50% cellulose, making it an important raw material for paper production and textile manufacturing (Haghanifar et al. 2020).

4. Agricultural Residues

Agricultural residues are a significant source of cellulose. These include crop residues like wheat straw, rice straw, corn stover as well as byproducts from food processing industries like sugarcane bagasse and citrus peels (Hou et al. (2020). These materials are often burned or discarded, but they can be used to produce bio fuels, paper and other products (Moreira et al. 2020).

5. Algae

Certain types of algae contain significant amounts of cellulose. These include green algae and blue-green algae, which are used as a source of bio fuels and other products (Moreira et al. 2020). Algae can be grown in large quantities in ponds or other controlled environments and can be harvested for their cellulose content.

6. Microorganisms

Certain types of bacteria and fungi produce cellulose as part of their cell walls. These microorganisms can be grown in large quantities and harvested for their cellulose content. Bacterial cellulose, in particular, has unique properties that make it useful in a variety of applications, including wound healing, tissue engineering, and food production (Rumi et al. (2021).

7. Municipal Solid Waste

Municipal solid waste (MSW) is another potential source of cellulose. MSW includes household and commercial waste and it typically contains a mix of organic and inorganic materials. The organic fraction of MSW can be processed to produce cellulose-based products like bio fuels, paper and textiles (Zhang (2017).

8. Seaweed

Certain types of seaweed contain significant amounts of cellulose. These include brown algae like Kelp, which are used as a source of bio fuels and other products. Seaweed can be grown in large quantities in the ocean and can be harvested for its cellulose content.

9. Microcrystalline Cellulose

Microcrystalline cellulose (MCC) is a refined form of cellulose that is produced by breaking down cellulose fibers into small, uniform particles. MCC is used as a bulking agent, binder, and disintegrant in pharmaceuticals, food products and cosmetics. It is also used as filler in tablets and capsules.

10. Recycled Paper

Recycled paper is an important source of cellulose. When paper is recycled, it is typically processed to remove inks, coatings, and other contaminants. The resulting pulp can be used to produce new paper products, as well as other cellulose-based products like insulation and packaging materials.

11. Textile Waste

Textile waste, including clothing and other fabric scraps, is a potential source of cellulose. These materials can be processed to produce new textile products or other cellulose-based products like paper and packaging materials.

12. Animal-based sources

While cellulose is primarily found in plant-based materials, certain animal-based sources also contain small amounts of cellulose(Jorfi & Foster 2014). These include the shells of crustaceans like shrimp and lobster as well as the feathers and hooves of animals.

Cellulose is a versatile and abundant natural polymer that is used in a wide range of applications (Barud et al. 2016). As new technologies are developed for processing and refining cellulose, it is likely that cellulose-based products will become even more important in the future

Organic Solar Cells

Organic solar cells, also known as organic photovoltaics (OPVs), are a type of solar cell that utilizes organic materials to convert sunlight into electricity. Unlike traditional solar cells based on inorganic semiconductors like silicon, organic solar cells employ organic molecules or polymers for several purposes.

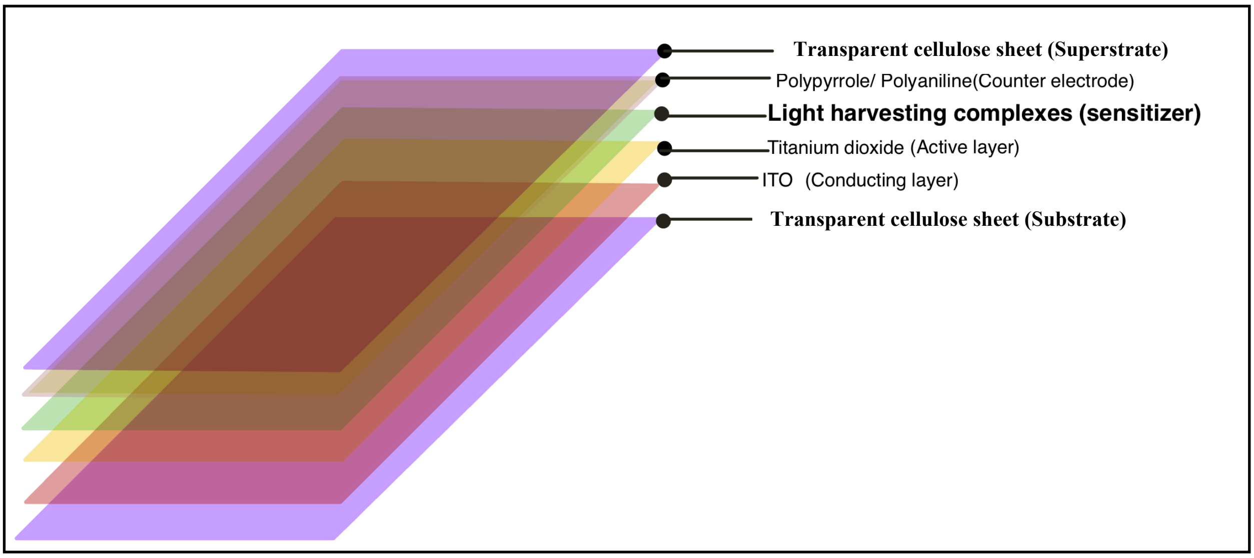

Figure 4: Devise Structure

1. Substrate and Superstrate

These can be of glass or a flexible substrate, such as a plastic or metal foil, to enable lightweight and flexible device fabrication. The active layer is deposited on the substrate.

In the present study, the substrate and superstrate have been made by using Cellulose.

Chapter 1

2. Conducting layer

Organic solar cells require transparent electrodes to allow light to pass through. The charge carriers are finally collected at these layers. Commonly used transparent electrode materials include Indium Tin Oxide (ITO) and more recently, flexible and transparent conductive polymers like PEDOT:PSS are being used.

In the present study also, Indium Tin Oxide (ITO) layer has been deposited the on the substrate and superstrate.

Chapter 2

3. Active layer

The active layer of an organic solar cell consists of a blend of electron-donating and electron-accepting inorganic or organic semiconducting material. These materials have complementary energy levels, allowing efficient charge separation and transport.

In the present study, Titanium Dioxide (TiO_2) layer has been used as the active material.

Chapter 3

4. Sensitizer

It is a layer that is meant to absorb additional light, resulting into charge carriers which enhance the photo current.

In the present study, plant based light harvesting complexes have been used as Sensitizers.

Chapter 4

5. Counter electrode

The counter electrode is meant to complete the circuit and allow charge to flow. Conventionally, metallic or carbon-based layers are used for counter electrodes. Polymers are also used for the purpose.

In the present study, Polypyrrole and Polyaniline have been used as Counter electrodes.

Chapter 5

6. Device formulation

Layers of material mentioned above were deposited to make the solar cells and their characteristics were studied.

Device formulation and study of characteristics.

Chapter 6

Advantages of organic solar cells:

1. **Flexibility:** Organic solar cells can be fabricated on flexible substrates, enabling the production of flexible and lightweight solar panels. This flexibility opens up new possibilities for applications, such as integration into curved surfaces or wearable devices.
2. **Low-Cost Manufacturing:** Organic solar cells can be manufactured using solution-based techniques such as printing or coating, which are potentially cheaper and scalable compared to traditional semiconductor processing methods.
3. **Energy Payback Time:** Organic solar cells have a relatively short energy payback time, meaning they can generate much more energy over their lifetime than the energy required to manufacture them. This is due to the low embodied energy of organic materials and the potential for low-cost manufacturing.
4. **Aesthetics:** Organic solar cells can be fabricated in various colors and designs, allowing for architectural integration and aesthetic customization.

CURRENT STATE OF RESEARCH IN ORGANIC SOLAR CELLS:

Research in organic solar cells is an active and rapidly evolving field. Scientists and engineers are continuously working to improve the efficiency, stability, and scalability of organic solar cell technology (Kang et al. 2008). Key areas of research include:

1. **Material Development:** Researchers are exploring new organic semiconductor materials with improved light absorption, charge transport and stability properties. This includes the development of novel conjugated polymers, small-molecule organic semiconductors and non-fullerene acceptor materials (Duché et al. 2009).
2. **Device Architecture:** Various device architectures, such as single-junction, tandem, and multi-junction configurations, are being investigated to enhance the power conversion efficiency and spectral response of organic solar cells (Shen et al. 2007).
3. **Stability and Lifetime:** Enhancing the stability and lifetime of organic solar cells is a critical research area. Efforts are focused on improving the materials' resistance to degradation from exposure to light, heat, moisture and oxygen to ensure long-term performance (Kesters et al. 2015).
4. **Upscaling and Manufacturing:** Researchers are working on improving the scalability and manufacturability of organic solar cells (Wang et al. 2009). This includes the development of roll-to-roll printing and coating techniques, as well as the optimization of device fabrication processes (Singh & Nalwa 2015).

EFFICIENCY ACHIEVED IN ORGANIC SOLAR CELLS:

The power conversion efficiency of organic solar cells has steadily increased over the years, reaching record values in the laboratory. As of September 2021, the highest reported power conversion efficiency for single-junction organic solar cells was around 18-19% (Zheng et al). However, it's important to note that efficiency values can vary depending on the specific materials and device architectures used in different studies.

In recent years, significant progress has been made in improving the efficiency of organic solar cells. This has been achieved through various approaches, including the development of new materials, device architectures, and optimization of fabrication processes (Li et al. 2015). Researchers have focused on enhancing light absorption, charge transport, and charge separation within the active layer of the solar cell (Sandberg et al. 2019).

One major area of research has been the development of non-fullerene acceptor materials. Fullerene derivatives, such as PCBM {[6,6]-phenyl-C_{61}-butyric acid methyl ester}, have been widely used as electron acceptors in organic solar cells (Hou et al. 2018). However, non-fullerene acceptors have emerged as promising alternatives due to their potential for higher efficiency and better stability (Meng et al. 2015). These materials have shown improved absorption characteristics and higher charge mobility, leading to enhanced device performance.

Tandem and multi-junction architectures have also gained attention in the research community (Sun et al. 2015). By combining multiple sub cells with complementary absorption spectra, these architectures aim to harvest a broader range of sunlight, thereby increasing the overall efficiency of the solar cell. Tandem devices can be achieved by stacking two or more sub cells, each optimized for a specific portion of the solar spectrum.

Stability and lifetime improvement have been another focus of research. Organic solar cells are generally more susceptible to degradation compared to their inorganic counterparts (Sutton et al. 2016). Efforts have been made to develop more stable materials and device structures, as well as encapsulation techniques to protect the active layer from environmental factors (Uddin et al. 2019). Stability testing under various conditions, including light, heat, and humidity, is conducted to assess the long-term performance of organic solar cells(Woo et al. 2021).

Upscaling and manufacturing of organic solar cells have also been actively investigated. Roll-to-roll printing and coating techniques, which allow for large-scale production, have been explored to reduce manufacturing costs and increase throughput (Hwang et al. 2015, Lee et al. 2020). Additionally, advancements in device architecture and fabrication processes have aimed to improve the reproducibility and yield of organic solar cell manufacturing (Liu et al. 2019).

It's worth noting that the efficiency of organic solar cells reported in research publications may not always translate to commercial products (Pivrikas et al. 2007, Onge et al. 2018). The reported efficiency values are typically obtained under optimized laboratory conditions and may not be representative of the performance of large-scale, commercially viable devices (Pourjafari et al. 2022, Brooks & Nazeeruddin 2021). However, the continuous advancements in organic solar cell technology and the growing number of research efforts indicate the potential of this technology for future energy applications (Du et al. 2022, Rakocevic et al. 2020).

Instrumentation

UV-VIS SPECTROSCOPY

UV-Vis analysis was performed on Thermo Fisher evolution 300 series. Instrument is shown below with the path of beam.

Figure 5: UV-Vis Spectrophotometer

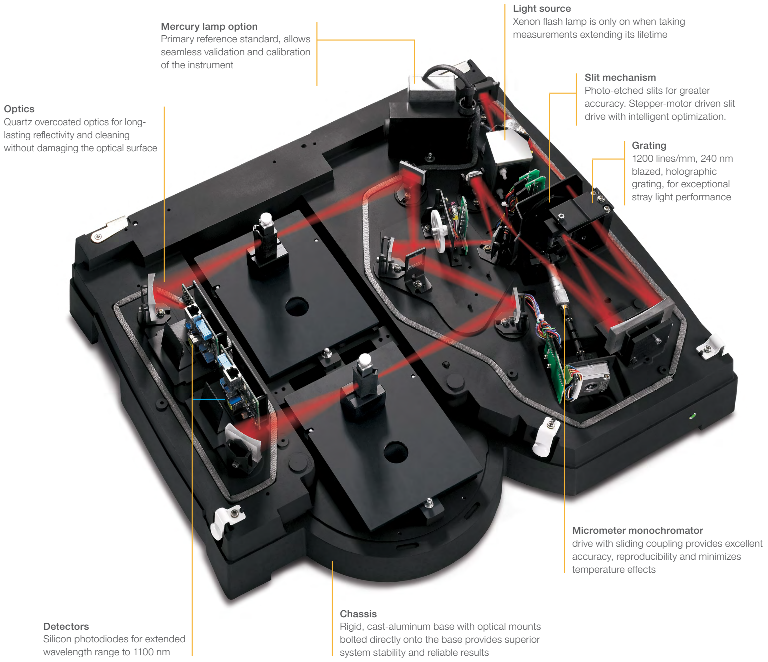

Figure 6: Optical Path in UV-Vis Spectrophotometer

UV-Vis spectroscopy, also known as ultraviolet-visible spectroscopy, is a widely used analytical technique for the qualitative and quantitative analysis of a wide range of compounds. This technique is based on the absorption or reflection of light by molecules in the UV and visible regions of the electromagnetic spectrum. UV-Vis spectroscopy is a non-destructive, fast, and accurate method of analysis that can be used in many fields such as chemistry, pharmaceuticals, environmental science, and materials science.

The UV-Vis spectrum of a sample can provide information about the electronic structure of the sample, the concentration of the sample, and the identity of the sample. The absorption or reflection of light by a sample is measured by the UV-Vis spectrophotometer, which can provide a quantitative measure of the sample's properties.

The principle of UV-Vis spectroscopy is based on the Beer-Lambert law, which states that the absorbance of a sample is directly proportional to the concentration of the sample and the path length of the incident light through the sample. The Beer-Lambert law can be expressed as:

$$\mathbf{A = \varepsilon c l}$$

where A is the absorbance of the sample, ε is the molar absorptivity, c is the concentration of the sample, and l is the path length of the incident light through the sample.

UV-Vis spectroscopy works by passing a beam of monochromatic light through a sample and measuring the amount of light absorbed or reflected by the sample. The UV-Vis spectrophotometer measures the intensity of the incident light before and after it passes through the sample, and the difference in the intensity is used to calculate the absorbance of the sample.

The Tauc relation is an empirical formula that relates the absorption coefficient of a semiconductor material to its band gap energy. It is given by:

$$\boldsymbol{\alpha(E) = A(E - Eg)^n}$$

where α is the absorption coefficient, E is the photon energy, Eg is the band gap energy, A is a constant, and n is an exponent that depends on the nature of the electronic transition involved. In general, n is taken to be either 1/2 or 2, depending on whether the transition is a direct or indirect allowed transition.

The absorption coefficient, α, is a measure of the rate at which light is absorbed by a material. It is related to the material's optical properties, and can be measured experimentally using techniques such as UV-Vis spectroscopy.

The band gap energy, Eg, is a fundamental property of a semiconductor material. It represents the energy required to promote an electron from the valence band to the conduction band, and is a key determinant of the material's electrical and optical properties.

The Tauc's relation can be used to estimate the band gap of a semiconductor material by measuring its absorption coefficient over a range of photon energies and fitting the data to the equation above. By extrapolating the data to zero absorption, the band gap energy can be determined.

It should be noted that the Tauc relation is an empirical formula, and its applicability depends on the nature of the electronic transitions involved in the absorption process. It may not provide accurate results for all materials, and other methods, such as density functional theory (DFT) calculations, may be required for more accurate band gap determination.

X-RAY DIFFRACTION ANALYSIS


Figure 7: XRD Instrument

XRD Analysis was performed on Regaku Smart lab SE series. The principle of XRD is based on the diffraction of X-rays by crystals. When X-rays are directed at a crystal, they are diffracted by the crystal lattice. The diffracted X-rays interfere constructively and destructively, producing a pattern of bright and dark spots on a detector. The XRD experiment involves directing a beam of X-rays at a sample and measuring the intensity of the diffracted X-rays at different angles. The angle of diffraction corresponds to the spacing between the crystal planes in the sample. The intensity of the diffracted X-rays is proportional to the number of atoms in the

The XRD pattern obtained from a sample provides information about the crystal structure, chemical composition, and physical properties of the material.

Bragg's law is a fundamental principle in X-ray diffraction (XRD) that allows for the determination of the crystal structure of a material. Bragg's law states that when X-rays are diffracted by a crystal, the diffraction angles (θ) satisfy the relationship:

$$n\lambda = 2d \sin \theta$$

where n is an integer, λ is the wavelength of the X-rays, d is the spacing between the crystal planes, and θ is the angle of diffraction.

In XRD, a beam of X-rays is directed at a crystal, and the diffracted X-rays are detected at different angles. By measuring the diffraction angles and using Bragg's law, the spacing between the crystal planes can be determined, which provides information about the crystal structure of the material. The peaks obtained in XRD graphs can then be analyzed using JCPDS data. The peaks obtained can be compared with JCPDS data and the exact structure of the crystal can be analyzed.

VISCOMETER

The principle of viscometry is based on the relationship between the shear stress and the shear rate of a fluid, which is described by the constitutive equation of the fluid. The constitutive equation relates the shear stress τ to the shear rate γ as follows:

$$\tau = \eta\gamma$$

where η is the viscosity of the fluid. The viscosity is a measure of the internal friction or resistance to flow of the fluid, and depends on the molecular structure, size, shape, and concentration of the molecules or particles in the fluid. For a Newtonian fluid, the viscosity is constant at different shear rates, and the constitutive equation is linear. For a non-Newtonian fluid, the viscosity is variable at different shear rates, and the constitutive equation is nonlinear.

WORKING:

The working of a viscometer depends on the type of viscometer used. In general, the working of a viscometer involves the following steps:

1. Sample preparation: The fluid sample is prepared by filtering, degassing, or stirring to ensure homogeneity and uniformity of the properties.
2. Calibration: The viscometer is calibrated using a reference fluid of known viscosity and temperature, or a standard calibration fluid provided by the manufacturer. The calibration ensures the accuracy and traceability of the measurements.
3. Measurement: The fluid sample is loaded into the viscometer, and the measurement is initiated by starting the motor or the timer. The shear rate or the shear stress is controlled by adjusting the speed or the torque, and the temperature is monitored and controlled by the temperature sensor and the control unit. The measurement is repeated several times to ensure reproducibility and consistency.
4. Data analysis: The measured values of torque, speed, time, and temperature are recorded and processed using software or firmware provided by the manufacturer. The software or firmware calculates the viscosity of the fluid using the rheological model and the geometrical and kinematic properties of the viscometer and the fluid. The results are displayed on the screen or stored in a database for further analysis and interpretation.

RF-MAGNETRON DEPOSITION UNIT

Figure 8: RF Magnetron Sputtering Unit

The basic principle of Rf magnetron sputtering can be explained as follows. A target material is placed in a vacuum chamber, and a gas, such as argon, is introduced into the chamber. A high-frequency RF power is applied to a cathode, which generates a magnetic field that traps electrons near the target surface. The trapped electrons ionize the gas atoms, creating a plasma of ions and electrons. The positive ions in the plasma are accelerated towards the negatively charged target surface, causing the ejection of atoms from the target material. These ejected atoms then travel through the vacuum chamber and deposit on a substrate to form a thin film.

The instrument used for RF Magnetron Sputtering was BOC Edwards Auto 500 RF with Indium Tin Oxide slab of diameter 3 inch and 1cm thickness. Argon gas was allowed to flow at a rate of 2 sccm.

PARTICLE SIZE ANALYZER

Shimadzu particle size analyzers use the principle of dynamic light scattering (DLS) to measure the size distribution of particles in a sample. The basic construction of a Shimadzu particle size analyzer consists of a laser source, a sample cell, a detector, and a data analysis system.

The working principle of the Shimadzu particle size analyzer is based on the fact that when a laser beam is passed through a sample containing dispersed particles, the particles will scatter light in all directions. The scattered light is then detected by a detector, which measures the intensity of the scattered light at different angles.

The size of the particles in the sample can be calculated from the intensity and the angular distribution of the scattered light using the Mie theory of light scattering. The Mie theory describes the scattering of light by particles of different sizes and refractive indices.

The Shimadzu particle size analyzer uses a dynamic light scattering technique, which means that the intensity of the scattered light is measured over time as the particles in the sample are undergoing Brownian motion. The Brownian motion of the particles causes fluctuations in the intensity of the scattered light, which can be analyzed to obtain information about the size distribution of the particles.

The sample cell in a Shimadzu particle size analyzer is typically a cuvette with a small volume of sample. The laser beam is passed through the sample cell, and the scattered light is detected at a range of different angles. The data analysis system then calculates the particle size distribution based on the intensity and angular distribution of the scattered light.

Figure 9: Particle Size Analyzer