SRI VENKATESWARA INTERNSHIP PROGRAM FOR RESEARCH IN ACADEMICS (SRI-VIPRA)

SRI-VIPRA

Project Report of 2024: SVP-2449

"Computational Studies on some organic and inorganic compounds for photo-voltaic applications"

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Sri Venkateswara College
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SRIVIPRA PROJECT 2024

Title : Computational Studies on some organic and inorganic compounds for photo-voltaic applications

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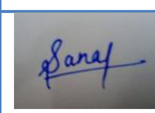
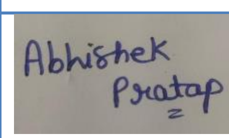
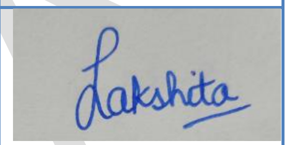
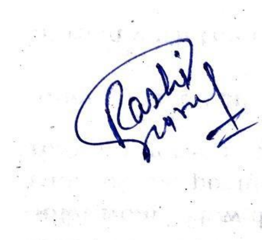
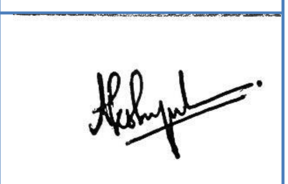
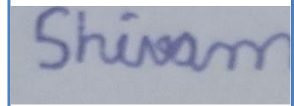
1		Sana Singh	1623016	BSc(H) Electronics	
2		Abhishek Pratap Singh Arya	1623043	BSc (H) Electronics	

					
3		Lakshita	1623049	BSc (H) Electronics	
4		Rashi Sharma	1623055	BSc.(H) Electronics	
5		Akshayah M	1123165	BSc. Life science (P)	

6		Shivam raj	1623046	B.sc electronics	

Signature of Mentors

Certificate of Originality

This is to certify that the aforementioned students from Sri Venkateswara College have participated in the summer project SVP-2449 titled "**Computational Studies on some organic and inorganic compounds for photo-voltaic applications"**. The participants have carried out the research project work under our guidance and supervision from 1st July, 2024 to 30th September 2024. The work carried out is original and carried out in an online/offline/hybrid mode.

Signature of Mentors

Acknowledgements

The authors would like to acknowledge Prof. Marc Burgelman (University of Ghent) for providing the simulation software SCAPS-1D.

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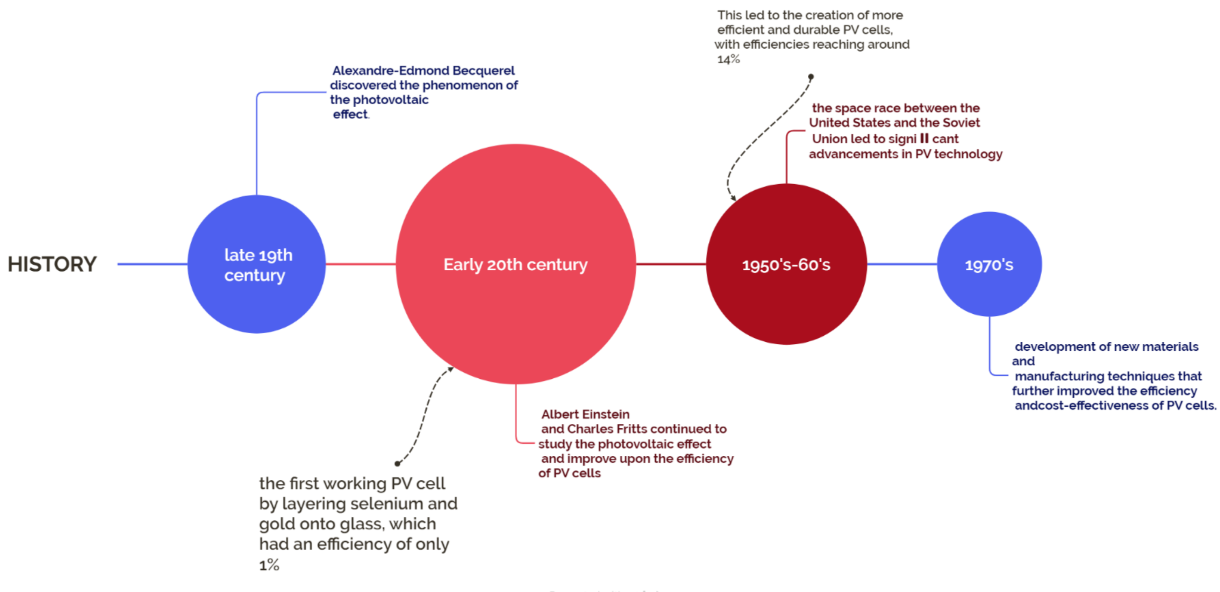
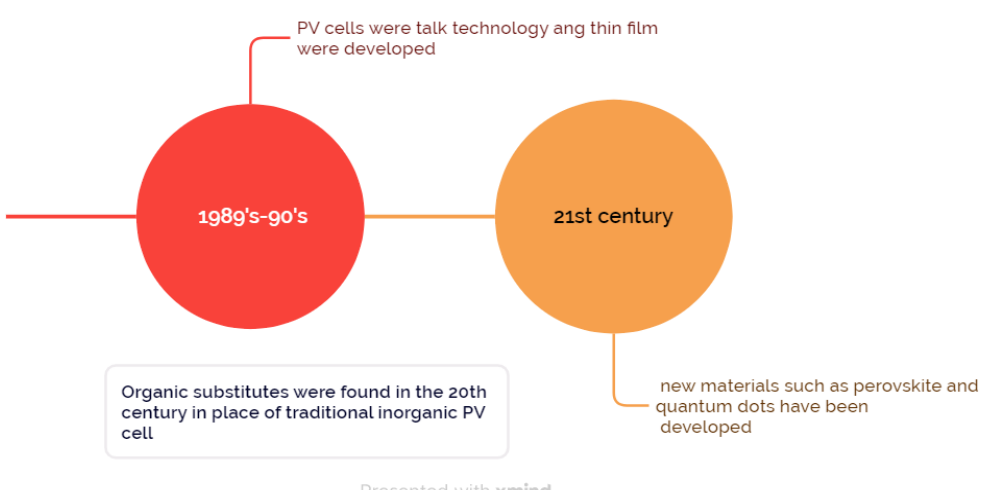
INTRODUCTION-:

Renewable Resources are essential for obtaining sustainable development, as it can provide limitless energy and resources for continuous growth of a society. It reduces dependency on fossil fuels, reduction in carbon emissions and promotes better environment friendly nature. One of the most affordable and abundant renewable resources is sunlight i.e Solar energy. It harnesses the sun's vast power to generate electricity through photovoltaic cells or solar thermal systems. It provides a clean, inexhaustible energy source which can be deployed globally, from large scale solar farms to individual rooftop panels without any harmful emissions. It even promotes lower electricity costs, and transition to a low-carbon economy, which will lead to resilient infrastructure for upcoming generations.





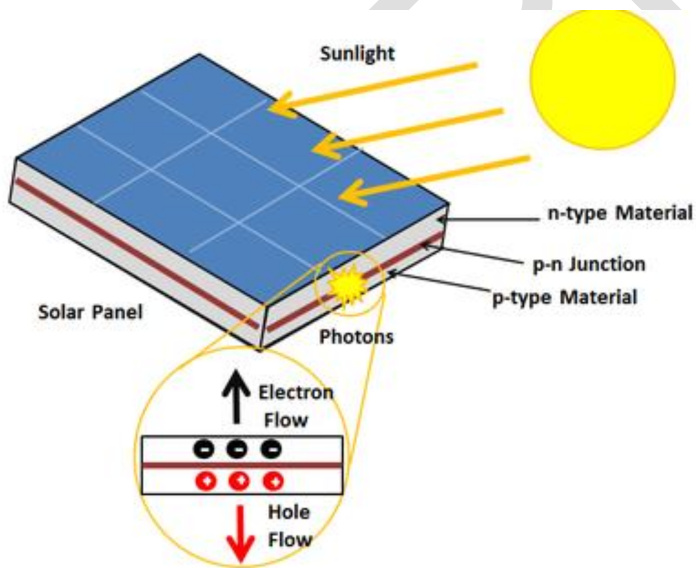
1. **Photovoltaic cell**

Photovoltaic cell is a device that converts solar energy into electrical energy through the photovoltaic effect. In this process the light photons get absorbed by the material which then generate electric energy.

1.1. **Fundamental principle of Photovoltaic cell:**

Photovoltaic effect:

The photovoltaic effect is the process in which voltage or electric current generates in a photovoltaic cell when exposed to sunlight. These solar cells are consist of two type of semiconductor p-type and n-type which combine to form a p-n junction. An electric field is formed in the region of junction as electron move to positive p side and holes move to negative n side. This causes the movement of electron and holes. When light of suitable wavelength is incident on the cell energy of the photon transferred to electrons causing it to jump to conduction band which lead to flow of electric current.



Photovoltaic Effect

2. **Photovoltaic Solar Cells:**

Photovoltaic (PV) solar cells have become a pivotal technology in the transition to renewable energy sources.

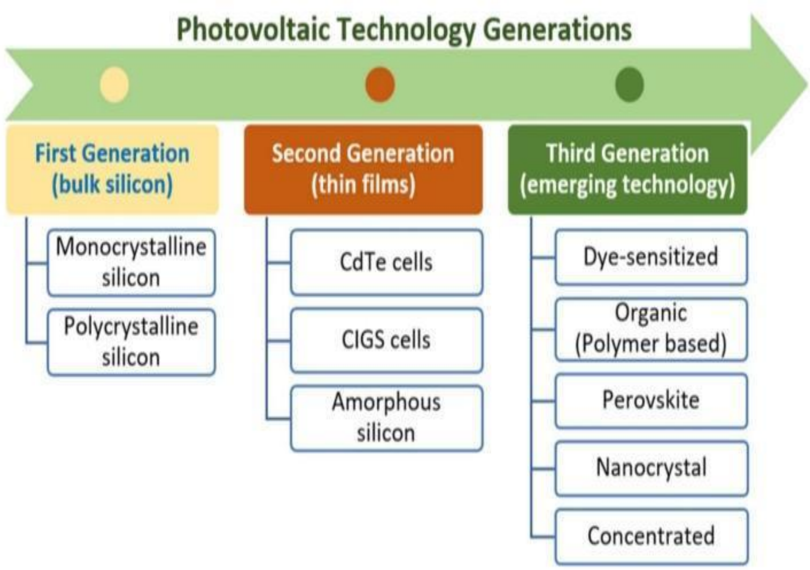
Emphasis is placed on recent research developments aimed at improving efficiency, reducing costs, and expanding the applicability of PV technology. They offer a sustainable solution to the growing global energy demand while reducing greenhouse gas emissions. The development and optimization of PV technologies are essential for achieving higher efficiencies and lower costs.

3. Types of Photovoltaic Cells:

i. Monocrystalline Silicon Cells
ii. Polycrystalline Silicon Cells
iii. Thin-Film Solar Cells
iv. Perovskite Solar Cells
v. Organic Photovoltaic Cells (OPV)

4. Generation of photovoltaic cells:

In the context of photovoltaic cells, "generation" refers to the different stages or categories of technological development that solar cells have undergone over time. These generations are typically categorized based on the materials and technologies used, as well as their efficiency, cost, and application characteristics.



4.1. Difference between three generations:

	First generation	Second generation	Third generation
Materials	Silicon	CIGS, CdTe, a-Si	Multi-junction cells, organic materials, perovskite materials, flexible substrates
Efficiency range	6–25%	10–15%	>25%
Advantages	Proven technology, increasing efficiency	Flexible, lightweight, roll-to-roll production, cost-effective	Cheaper materials, potential to significantly reduce the cost of solar energy, higher efficiencies
Limitations	High raw material cost, performance drops in high temperatures	Lower efficiency, long-term stability and durability, not yet well understood	Still in the research and development phase
Manufacturing process	Wafer-based	Roll-to-roll	Various, depending on material and design
Applications	Residential, commercial, utility-scale projects	Building-integrated photovoltaics, portable and lightweight solar panels, small-scale projects	Large-scale projects, consumer electronics, off-grid applications
Durability	Good	Moderate	Varies, depending on material and design
Stability	Good	Moderate	Varies, depending on material and design

5. Solar PV technology and Materials

C-Si- Crystalline Silicon Solar Systems are generally constructed from two essential types of

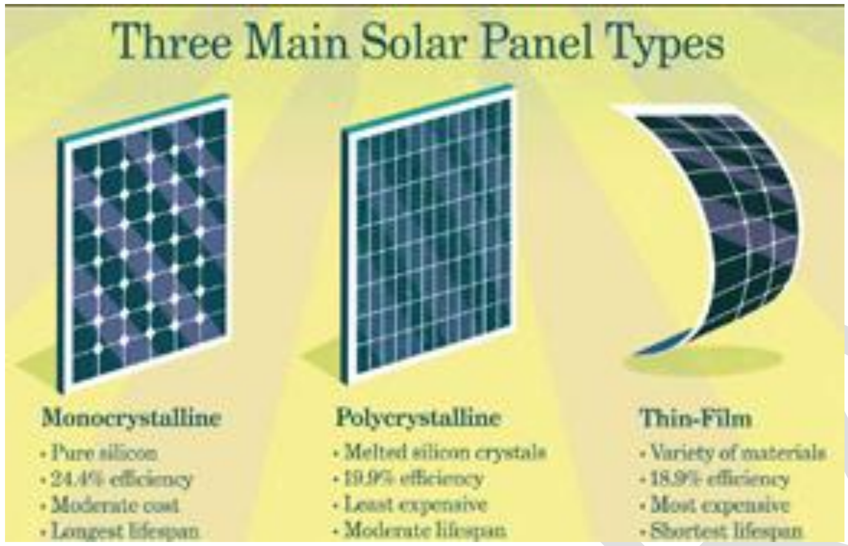
Crystalline structures: Monocrystalline and Multicrystaline.

The Monocrystalline structures offer 20% better efficiency than multicrystalline ones but are more expensive. The technologies which are used to create the photovoltaic cells are-:

- C-Si (Crystalline Silicon) Wafer -Based technology
- A-Si (Amorphous Silicon) thin film technology.

The C-Si wafer based technology is quite costly, while thin- film technology is comparatively cheaper and cost effective.

The Cell- Efficiency of thin-film technology varies from 5% to 7%, and with double and triple junction, it can increase to 8% to 10%.



6. Organic Photovoltaic Cells

Organic photovoltaic (OPV) cells have attracted considerable interest due to their potential for cost-effective, large-scale production and unique physical properties. OPV cells utilise organic molecules or polymers as the active layer for light absorption and charge transport, differentiating them from traditional silicon-based PV cells**.**

Working Principles of OPV Cells-:

● Absorption of light-: In OPV cells, organic materials absorb photons, generating electron-hole pairs. Efficient light absorption depends on the material's structure, molecular weight, and orientation. Strategies like conjugated polymers, optimized morphology, light-trapping structures, and plasmonic nanoparticles enhance absorption, improving charge separation and transport, ultimately boosting OPV cell efficiency.

● Charge Separation-: Electron hole pairs are separated by a built in electric field created by the energy difference between donor and acceptor materials in the active layer. Efficient charge separation occurs at the donor-acceptor interface, with morphology playing a crucial role. This can be enhanced by using material alignment, using alternative acceptors like non-fullerene, and employing tandem structures for improved exciton dissociation and overall efficiency.

● Charge Collection-: Now, the separated electrons and holes are collected by electrodes made of transparent conductive materials like ITO, aluminum, or silver. Efficient charge collection, crucial for device performance, depends on active layer morphology, charge carrier mobility, and proper energy level alignment between donor and acceptor materials.

● Electrical Output-: The electrical output of the cell depends on charge separation and collection efficiency. Key performance metrics include short-circuit current density, open-circuit voltage, fill factor, and power conversion efficiency. These factors collectively decide the efficiency of the organic photovoltaic cell.

6.1 Materials used in Organic Photovoltaic cells (OPV)

The efficiency of OPV cells depends heavily on the materials used, which include:

1. Donor Materials
2. Acceptor Materials
3. Electrodes

6.1.1 Role of Polyaniline in Organic photovoltaic cells

The global push for sustainable energy sources has led to increased interest in renewable technologies, particularly in solar energy conversion. Organic photovoltaics (OPVs) offer a lightweight, flexible, and potentially low-cost alternative to traditional silicon-based solar cells. Among the various materials investigated, polyaniline stands out due to its unique combination of electrical conductivity, stability, and ease of processing. It is a conductive organic polymer that has many applications.

6.1.2 Properties of Polyaniline:

1.Electrical Conductivity:

PANI exhibits semiconductor-like properties. Which makes it suitable for charge transport in photovoltaic applications. Also it's electrical conductivity increases exponentially with increase in temperature.

2. Environment Stability:

PANI shows a high degree of stability against environmental degradation. Which makes this compound different from others.

3. Appearance:

PANI can be clear or colourless.

4. Thermal stability:

PANI has high thermal stability.

6.1.2 Integrating PANI into other OPV structures:

1.Spin Coating:

This technique provides a uniform thin film of PANI, allowing for precise control over layer thickness.

2. Layer by layer Assembly:

It is a method of coating substrates with polymers to improve their chemical and electrochemical stability.

3. Blending with other polymers:

Combining with other polymers including conductive or semiconductive can improve overall device performance.

Recent studies indicate that PANI-based OPV cells can achieve power conversion efficiencies (PCE) of 3% to 6%. Key performance metrics include:

1. Power Conservation Efficiency
2. Stability

7. Recent advancement in Photovoltaic cell

i. Advancement in PV technology have focused on improving efficiency of photovoltaic cell.
ii. Thin film technology and organic material offer low material cost contributing to low manufacturing cost.
iii. Day by day research are done to enhance the stability and durability of photovoltaic cell.

8. Advantages of OPV cell over PV cell:

i. Flexibility: OPVs are more flexible and lightweight than PV cell. The flexibility allows OPVs to be applied to a wide range of substrate such as plastic and glass.
ii. Low-cost manufacturing: OPVs use less silicon and using low temperature, etc.
iii. Lower energy consumption in production: The production of OPVs require less energy compared to silicon-based PV cell.

9. Challenges:

Organic photovoltaic (OPV) cells, while promising for their flexibility, low cost, and potential for large-area production, face several technical challenges:

i. **Efficiency**: OPV cells generally have lower power conversion efficiencies compared to inorganic counterparts like silicon-based solar cells.

ii. **Stability and Lifespan**: The materials used in OPV cells are often less stable than inorganic materials. They can degrade due to exposure to oxygen, moisture, and UV light, leading to shorter lifespans.

iii. **Material Purity and Processing:** High purity of organic materials is crucial for the performance of OPV cells, but achieving and maintaining this purity can be challenging.

iv. **Environmental Impact:** The long-term environmental impact of the materials used in OPV cells, including their production, use, and disposal, is not yet fully understood.

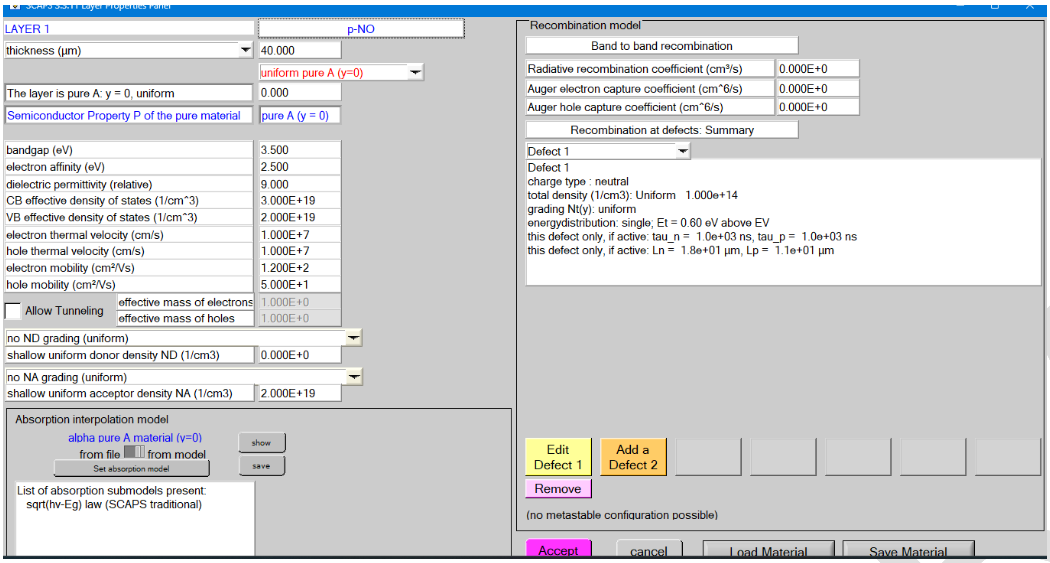
v. **Scaling and Manufacturing**: While OPV cells are potentially cheaper and easier to manufacture, scaling up production to industrial levels while maintaining quality and performance is a significant challenge.

10. Conclusion:

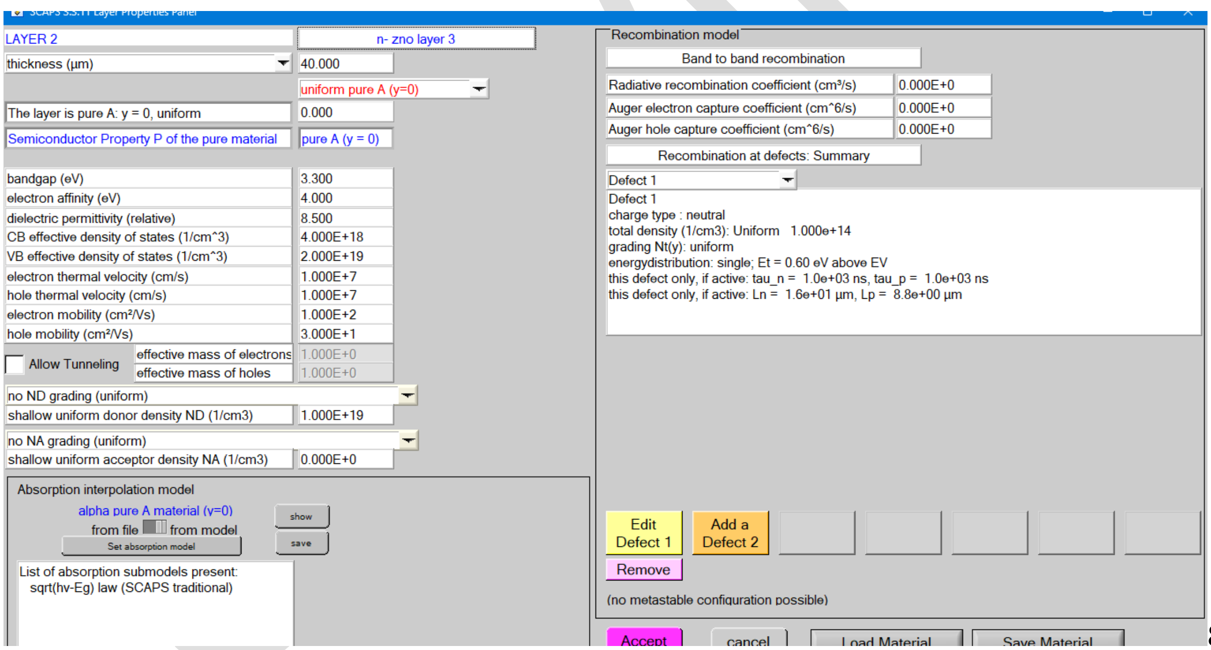
Photovoltaic cells have made significant strides in the renewable energy landscape. It has advances in material science, manufacturing techniques. However, challenges remain in developing sustainable, cost-effective, reliable and high efficiency. So, continued research will be crucial in the innovation of Photovoltaic cells.

Appendix I: Simulation of Solar Cells using SCAPS

1) When you open scaps then this window opens which contains many functions.
2) Here you can see (Dark/Light) option which help you to work your photovoltaic cell work in dark or in the exposure of light.
3) At bottom you can see the Set problem option, click on it.



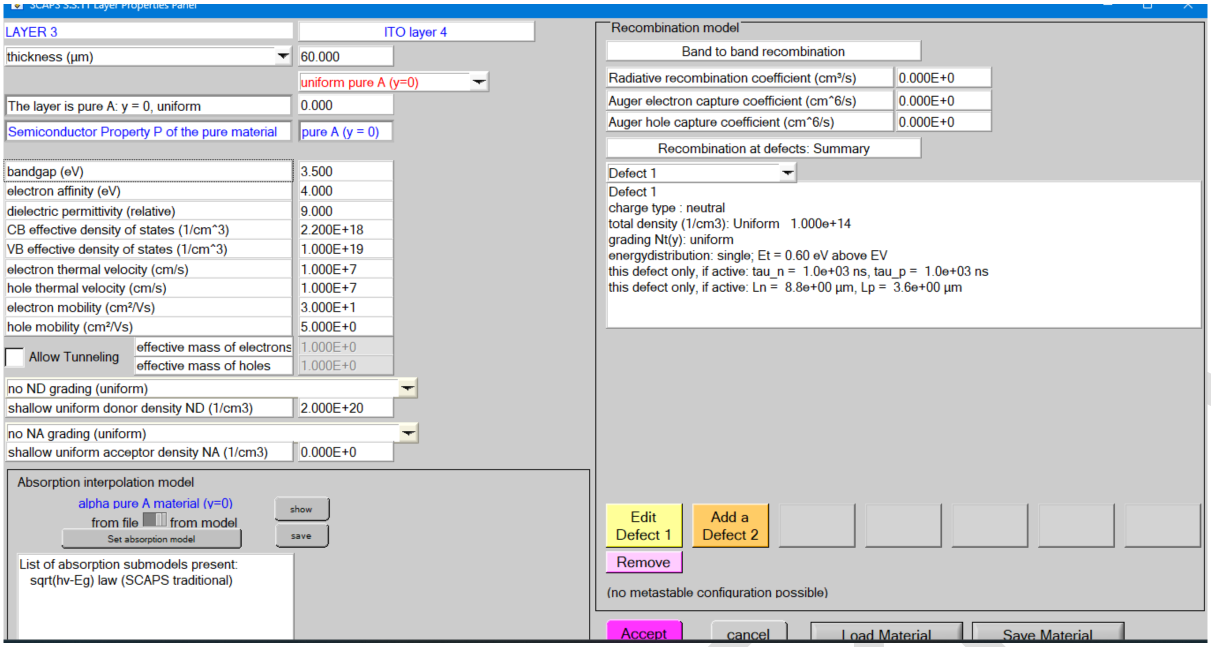
4) After clicking on the set problem option this display was opened.
5) Now make a layer material of your choice.
6) Now click on the defect option and then press on ok.
7) Then press on the accept option at the bottom of the window.



8) When you press add layer (n-zno), option then this window open.

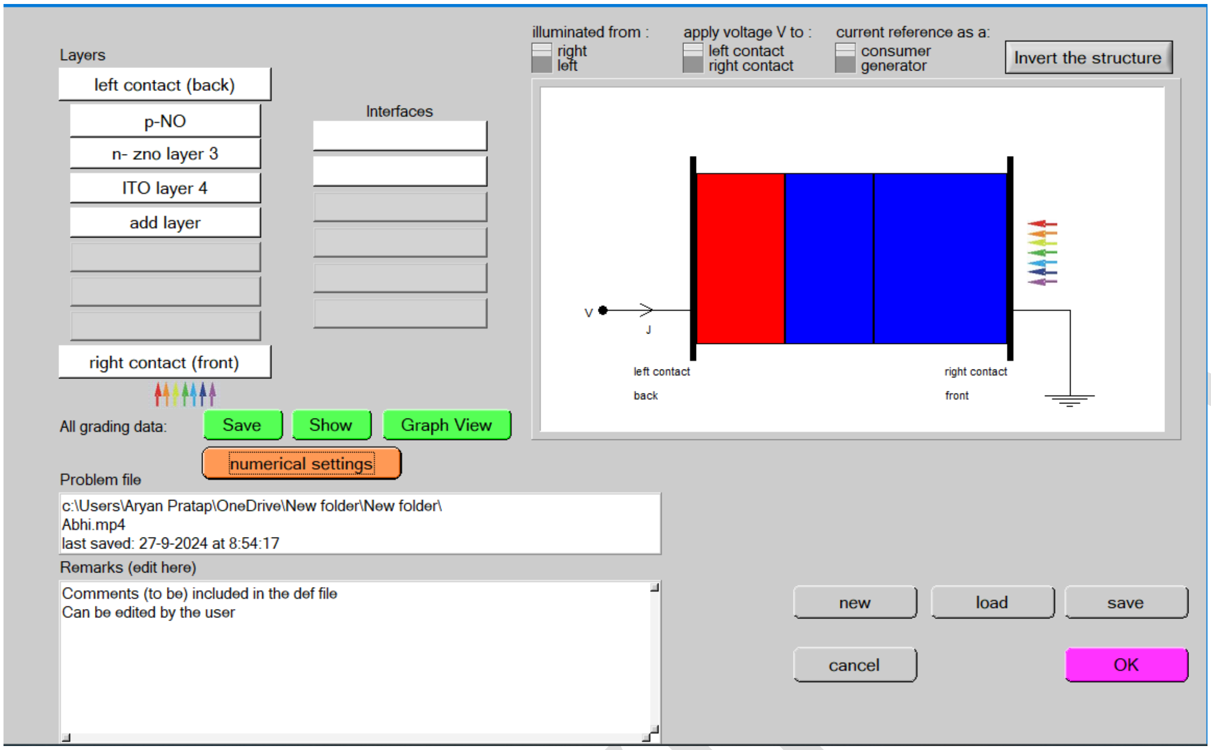
9) Now fill the information of layer second then click on edit defect option then click on accept option.

10) After that add a new ITO layer.



11) Now follow these options which you followed earlier and press on accept option.

12) After inserting all the layers you can see this window :-

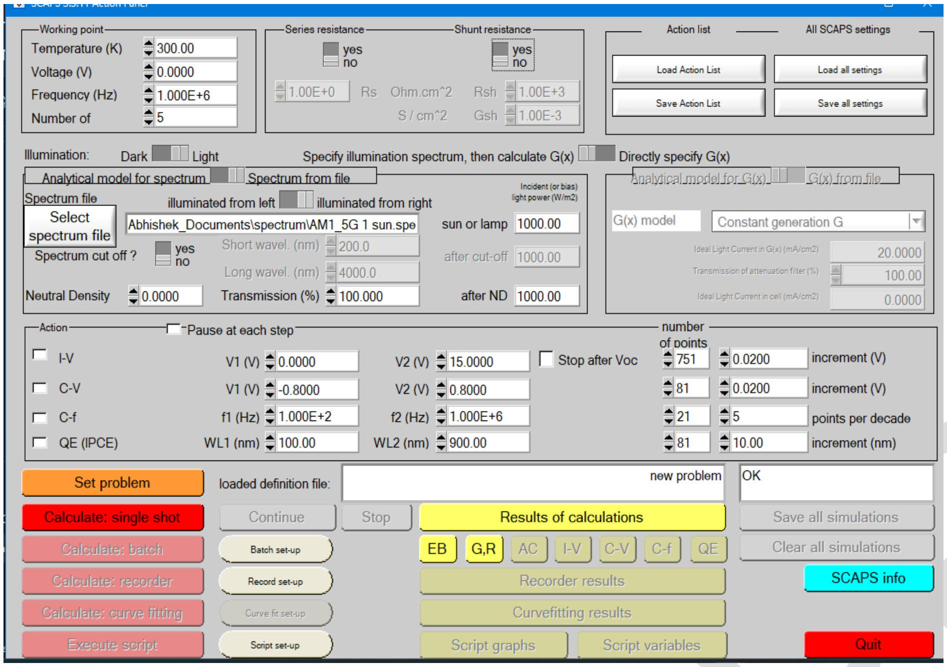


13) Here you can see all the layers which you inserted .

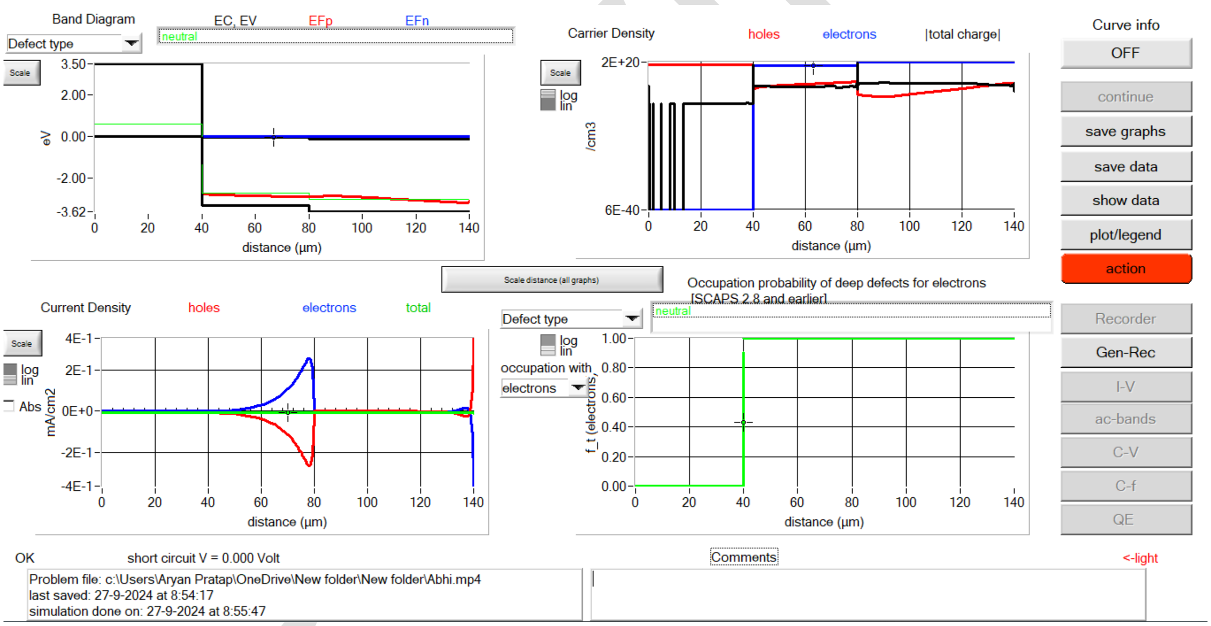
14) Now press on save option and save it.

15) Then press on the ok option.

16) This window will open on your screen.



17) Now click on the (calculate single shot) option and a output window open in front of you.



18) This window shows the output in terms of parameters like Band Diagram, Carrier Density, Current density and defects of your photovoltaic cell.

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