

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



SRI-VIPRA

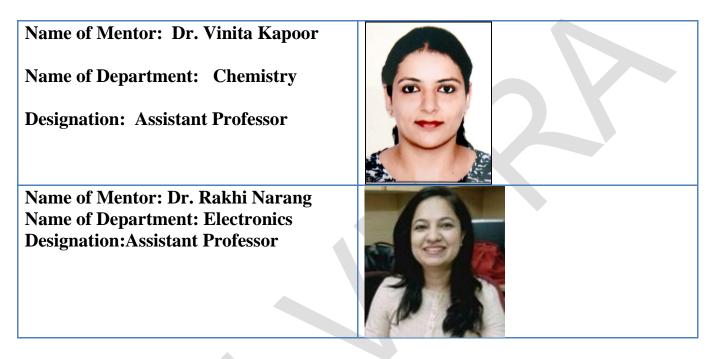
Project Report of 2024: SVP-2449

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

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SRIVIPRA PROJECT 2024

Title : Computational Studies on some organic and inorganic compounds for photovoltaic applications



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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

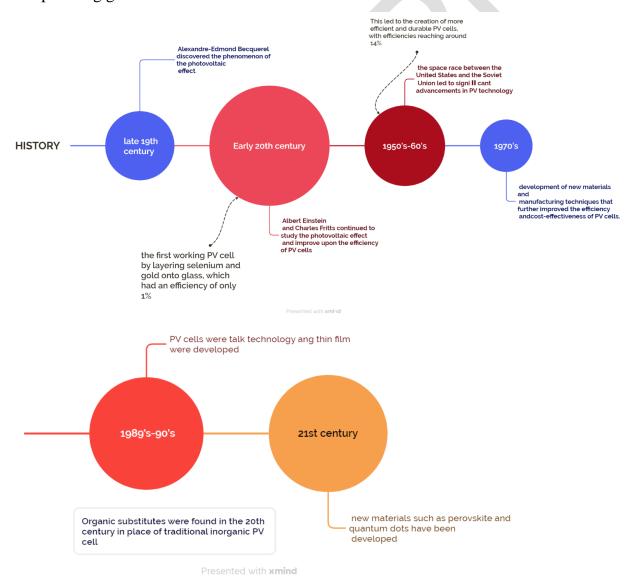
The authors would like to acknowledge Prof. Marc Burgelman (University of Ghent) for providing the simulation software SCAPS-1D.

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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.



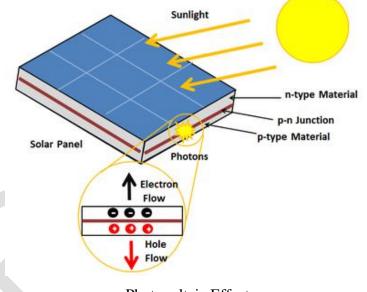
1. Photovoltaic cell

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.

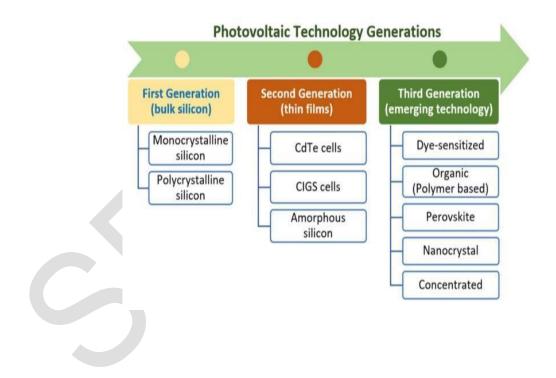
Emphasis is placed on recent research developments aimed at improving efficiency, reducing costs, and expanding the applicability of PV technology. They offer a sustainable solution to the growing global energy demand while reducing greenhouse gas emissions. The development and optimization of PV technologies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

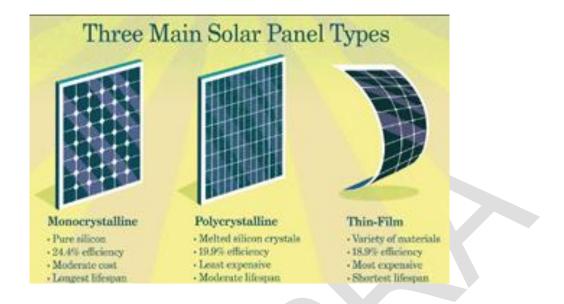
Crystalline structures: Monocrystalline and Multicrystaline.

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 costeffective, 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 largearea production, face several technical challenges:

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

- 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.

 SCAPS SISTE Layer Properties Parier 			
LAYER 1		p-NO	Recombination model
thickness (μm)	40.000		Band to band recombination
	uniform pure A	(y=0) 🖵	Radiative recombination coefficient (cm ² /s) 0.000E+0
The layer is pure A: y = 0, uniform	0.000		Auger electron capture coefficient (cm ^{-6/s}) 0.000E+0
Semiconductor Property P of the pure material	pure A (y = 0)	1	Auger hole capture coefficient (cm°6/s) 0.000E+0
,	1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2		Recombination at defects: Summary
bandgap (eV)	3.500		Defect 1
electron affinity (eV)	2.500		Defect 1
dielectric permittivity (relative)	9.000		charge type : neutral
CB effective density of states (1/cm^3)	3.000E+19		total density (1/cm3): Uniform 1.000e+14 grading Nt(v): uniform
VB effective density of states (1/cm^3)	2.000E+19		graung N(y), uniform energydistribution; single; Et = 0.60 eV above EV
electron thermal velocity (cm/s)	1.000E+7		this defect only, if active: tau_n = 1.0e+03 ns, tau_p = 1.0e+03 ns
hole thermal velocity (cm/s)	1.000E+7		this defect only, if active: Ln = 1.8e+01 μm, Lp = 1.1e+01 μm
electron mobility (cm²/Vs)	1.200E+2		
hole mobility (cm²/Vs)	5.000E+1		
Allow Tunneling			
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)	2.000E+19		
Absorption interpolation model			
alaba sure A material (u=0)	. 1		
from file from model	show		Edit Add a
	save		Defect 1 Defect 2
List of absorption submodels present:	1		Remove
sgrt(hv-Eg) law (SCAPS traditional)			
square 29, and (e.s. a o additional)			(no metastable configuration possible)
			Accept cancel Load Material Save Material

- 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.

LAYER 2	n- zno layer 3	Recombination model
thickness (μm) 🔻	40.000	Band to band recombination
	uniform pure A (y=0)	Radiative recombination coefficient (cm³/s) 0.000E+0
The layer is pure A: y = 0, uniform	0.000	Auger electron capture coefficient (cm^6/s) 0.000E+0
Semiconductor Property P of the pure material	pure A ($y = 0$)	Auger hole capture coefficient (cm^6/s) 0.000E+0
Semiconductor Property P of the pure material		Recombination at defects: Summary
bandgap (eV)	3.300	Defect 1
electron affinity (eV)	4.000	Defect 1
dielectric permittivity (relative)	8.500	charge type : neutral
CB effective density of states (1/cm ³)	4.000E+18	total density (1/cm3): Uniform 1.000e+14 grading Nt(y): uniform
VB effective density of states (1/cm ³)	2.000E+19	energydistribution: single; Et = 0.60 eV above EV
electron thermal velocity (cm/s)	1.000E+7	this defect only, if active: tau_n = 1.0e+03 ns, tau_p = 1.0e+03 ns
hole thermal velocity (cm/s)	1.000E+7	this defect only, if active: Ln = 1.6e+01 μm, Lp = 8.8e+00 μm
electron mobility (cm²/Vs)	1.000E+2	
hole mobility (cm²/Vs)	3.000E+1	
Allow Tunneling		
effective mass of holes	1.000E+0	
no ND grading (uniform)	-	
shallow uniform donor density ND (1/cm3)	1.000E+19	
no NA grading (uniform)		
shallow uniform acceptor density NA (1/cm3)	0.000E+0	
Absorption interpolation model		1
alpha pure A material (y=0)	show	
from file from model	, www.	Edit Add a
Set absorption model	save	Defect 1 Defect 2
List of absorption submodels present:		Remove
sqrt(hv-Eg) law (SCAPS traditional)		
		(no metastable configuration possible)
		Accept cancel Load Material Save Material
		Accept cancel Load Material Save Material

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.

SUAPS 5.5.11 Layer Properties Parier			
LAYER 3	ITO layer 4	Recombination model	1
thickness (μm)	60.000	Band to band recombination	
	uniform pure A (y=0)	Radiative recombination coefficient (cm³/s) 0.000E+0	
The layer is pure A: y = 0, uniform	0.000	Auger electron capture coefficient (cm^6/s) 0.000E+0	
Semiconductor Property P of the pure material	pure A ($y = 0$)	Auger hole capture coefficient (cm^6/s) 0.000E+0	
	participation of	Recombination at defects: Summary	
bandgap (eV)	3.500	Defect 1	
electron affinity (eV)	4.000	Defect 1	
dielectric permittivity (relative)	9.000	charge type : neutral	
CB effective density of states (1/cm^3)	2.200E+18	total density (1/cm3): Uniform 1.000e+14 grading Nt(y): uniform	
VB effective density of states (1/cm ³)	1.000E+19	energydistribution: single; Et = 0.60 eV above EV	
electron thermal velocity (cm/s)	1.000E+7	this defect only, if active: tau n = 1.0e+03 ns, tau p = 1.0e+03 ns	
hole thermal velocity (cm/s)	1.000E+7	this defect only, if active: Ln = 8.8e+00 μm, Lp = 3.6e+00 μm	
electron mobility (cm²/Vs)	3.000E+1		
hole mobility (cm²/Vs)	5.000E+0		
Allow Tunneling	s 1.000E+0		
effective mass of holes	1.000E+0		
no ND grading (uniform)	-		
shallow uniform donor density ND (1/cm3)	2.000E+20		
no NA grading (uniform)	-		
shallow uniform acceptor density NA (1/cm3)	0.000E+0		
Absorption interpolation model			
alpha pure A material (v=0)	. 1		
from file from model	show	Edit Add a	
Set absorption model	save	Defect 1 Defect 2	
List of absorption submodels present:		Remove	
sqrt(hv-Eg) law (SCAPS traditional)			
		(no metastable configuration possible)	
		Accept cancel Load Material Save Material	

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

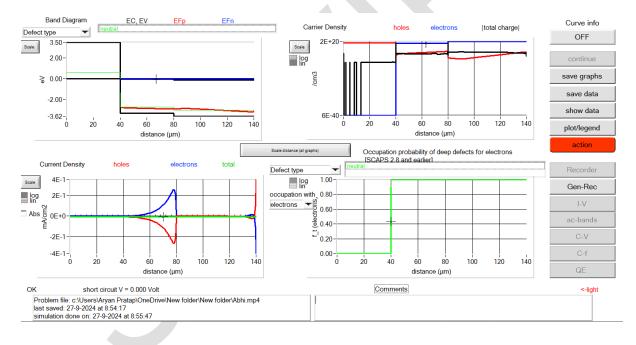
12) After inserting all the layers you can see this window :-

Layers	1	illuminated from : right left	apply voltage V to : left contact right contact	current reference as a: consumer generator	Invert the structure	
left contact (back)						
p-NO	Interfaces					
n- zno layer 3						
ITO layer 4						
add layer					*	
					₩ ₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩₩	
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		J				
right contact (front)		left cor	tact	right conta	act	
# ###################################	-	back		front	<u> </u>	
All grading data: Save	Show Graph View					
Problem file	erical settings					
c:\Users\Aryan Pratap\OneDr Abhi.mp4	ive\New folder\New folder\					
last saved: 27-9-2024 at 8:54	17					
Remarks (edit here)						
Comments (to be) included ir Can be edited by the user	n the def file		_	new loa	ad save	
				cancel	ОК	

- 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.

CALO DISTER ACUOIT UNCL				<u> </u>	
-Working point	Series resistance -	Shunt resistance	Action list	All SCAPS settings	
emperature (K) \$300.00 /oltage (V) \$0.0000	yes	yes no	Load Action List	Load all settings	
requency (Hz)		Ohm.cm^2 Rsh = 1.00E+3			
Number of \$		S / cm^2 Gsh 1.00E-3	Save Action List	Save all settings	
umination: Dark	ight Cossificillumi	nation spectrum, then calculate G(x) Directly specify G(x)		
Analytical model for spectrur			Analytical model for G	i(x) G(x) from file	
pectrum file illumi	nated from left	from right light power (W/r	(as) (as)		
Select pectrum file	ocuments\spectrum\AM1_5G 1 s	un.spe sun or lamp 1000.00	G(x) model Const	tant generation G	
Spectrum cut off ? yes		after cut-off 1000.00		nt in G(x) (mA/cm2) 20.0000	
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eutral Density = 0.0000	Transmission (%) 韋 100.00	0 after ND 1000.00	Ideal Light Curr	ent in cell (mA/cm2) 0.0000	
	ause at each step		of points		
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C-V	V1 (V) 🚔 -0.8000	V2 (V) 🖨 0.8000	\$81 €0.0	200 increment (V)	
C-f	f1 (Hz) 🖨 1.000E+2	f2 (Hz) 🖨 1.000E+6	\$21 \$5	points per decade	
QE (IPCE)	WL1 (nm) 🚔 100.00	VL2 (nm) 韋 900.00	€81 €10.	00 increment (nm)	
Set problem	loaded definition file:		new problem C	к	
Calculate: single shot	Continue St	op Results of	calculations	Save all simulations	
	Batch set-up		I-V C-V C-F QE	Clear all simulations	
	Record set-up	Record	er results	SCAPS info	
	Curve fit set-up	Curvefitt	ing results		
)		

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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