Optimization of non-leaded $KSnI_3$-based perovskite solar cells for performance enhancement using wxAMPS and SCAPS-1D simulation

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by

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CANDIDATE'S DECLARATION

We, Anjali Tyagi, (2K22/MSCPHY/03) and Dikhsa, (2K22/MSCPHY/11) hereby certify that the work which is presented in the Dissertation Project-II/Research work entitled "**Optimization of non-leaded $KSnI_3$-based perovskite solar cells for performance enhancement using wxAMPS and SCAPS-1D simulation**" in fulfillment of the requirement for the award of the degree of Master of Science in Physics and submitted to the Department of Applied Physics, Delhi Technological University, Delhi is an authentic record of our own, carried out during a period from August 2023 to May 2024, under the supervision of Dr. Sarita Baghel and Prof. Vinod SinghThe matter presented in this report/thesis has not been submitted by us for the award of any other degree of this or any other Institute/University. The work has been accepted for publication in peer-reviewed Scopus-indexed conference with the following details:

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Optimization of non-leaded $KSnI_3$-based perovskite solar cells for performance enhancement using wxAMPS and SCAPS-1D simulation

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ABSTRACT

The non-leaded perovskite material $KSnI_3$ is an excellent candidate for high-efficiency PSCs due to its exceptional electronic properties. It is robust, ductile in nature, and thermodynamically stable. These attributes make $KSnI_3$ as prominent perovskite material for the synthesis of highly efficient device. The device is simulated by using wxAMPS software and the results are validated by SCAPS-1D software. In this work, we have optimized various parameters like thickness of absorber layer, operating temperature, and electron affinity to get the maximum PCE. The maximum efficiency of 24.88% with FF=92.23%, V_{OC}=1.71 V, J_{SC}=13.20 mA/cm^2 is obtained for Cu_2O as HTL and ZnSe as ETL at an absorber layer thickness of 730 nm, and at temperature of 300 K. We have employed low-cost tungsten as a back contact for better efficiency and for low-cost device.

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LIST OF ABBREVIATION

Symbol/index	Meaning/Abbreviation
PCE	Power Conversion Efficiency
FF	Fill Factor
ETL	Electron Transport Layer
HTL	Hole Transport Layer
μ_e	Electron Mobility
μ_p	Hole mobility
N_D	Conduction band effective density of states
N_A	Valence band effective density of states
J_{SC}	Current density
V_{OC}	Voltage
$KSnI_3$	Potassium Tin Iodide

Chapter1
Introduction

1.1 BACKGROUND

The need for energy has grown significantly during the past few decades. To meet the energy needs, several energy sources have been used. Future energy needs could potentially be met by solar energy, which has shown to be a highly effective and efficient energy source. High-efficiency perovskite solar cells (PSCs) were developed using methyl ammonium lead halide perovskite structures as a visible light sensitizer [1]. They outperform other solar cells thanks to their best power conversion efficiency. If new tactics are implemented to increase the PSCs' long-term stability, they can be put to useful use. The optoelectronic characteristics of the perovskite materials, PSC construction, and current developments in electron transport layers for PSC production have all been covered in this chapter.

Sunlight is one of the main sources of solar energy that the world receives. To meet our energy needs, this sunshine can be transformed into electrical energy. Solar cells, a type of photovoltaic technology, are capable of directly converting sunlight into electricity. Numerous varieties of photovoltaic devices, including perovskite solar cells, polymer solar cells, organic solar cells (OSCs), DSSCs, and quantum-dot sensitized solar cells, were developed in earlier decades. Because of their low cost and simple manufacturing method, these kinds of solar cells have piqued the curiosity of scientists. PSCs sparked a lot of interest because of their excellent photovoltaic performance and reasonable pricing. One part of PSCs is a perovskite light absorber layer. The chemical formula of the material referred to as perovskite is ABO_3. The calcium titanate was referred to as a perovskite ($CaTiO_3$)[2]. There is also another type of perovskite materials that have the chemical formula ABX_3, where X = I−, Br−, or Cl−, and A= Cs+, CH_3NH_3. This particular class of perovskite materials has a reasonable band gap, good absorption qualities, and charge carrier properties.

1.2 INTRODUCTION

Perovskite have garnered attention due to the massive energy crisis of the twenty-first century, which has led to an exponential increase in the production of sustainable solar energy in recent years. There are three generations of SCs. High carrier mobilities are a feature of first-generation silicon solar cells (SCs), and the technology has advanced to the point where it may be used commercially [2].

Among the thin film cells that comprise the second generation of solar cells (SCs) are amorphous silicon (Si),CdTe, and CIGS. These cells have a lower PCE but are also less costly than silicon SCs [3]. Third-generation solar cells (SCs) are made up of perovskite, organic, and dye-sensitized solar cells (PSCs), which are unstable in the short term and lack

the technological maturity required for widespread usage in industry [4]. Science has been very interested in the performance of perovskite materials in solar cell devices. Lead halides that are hybridized from organic and inorganic materials possess a configurable bandgap, ease of synthesis, a high absorption coefficient, the ability to be processed in solutions, and extended diffusion lengths. They are promising materials for light absorbers in solar cells because of these qualities. The first organic-inorganic lead halide PSCs with an efficiency of 3.8% was reported in 2009 [5]. Recent efforts by the scientific community have resulted in its efficiency reaching 25.5%. The potentially dangerous lead component of the PSC has been one of the main barriers to its commercialization. Pb2+'s outer shell is similar to that of Ge2+ and Sn2+, two other divalent cations that have been examined. When Sn2+ and Ge2+ are used in place of Pb2+, there are no problems [6]. Anything of the general form ABX_3, on the other hand, is a perovskite structure. For the crystal cubic structure to be symmetrical, atom A must have a larger atomic radius and a lower electronegativity than atom B. Lead-free $KSnI_3$ has an affinity of 3.44 eV and a bandgap of 1.84 eV with 10.4 permittivity [7]. As a result, we need other lead-free perovskite absorbing layers, and $KSnI_3$ is a promising option for high-efficiency PSCs.The layer that promotes the passage of electrons while impeding the movement of holes is known as the electron transport layer (ETL) and the layer that impedes the movement of holes is known as the hole transport layer (HTL).

1.2.1 SOLAR ENERGY

One of the most important and efficient renewable energy sources is solar energy.One naturally replenishing renewable energy source is solar energy.
Since solar energy is unaffected by fossil fuels, it is environmentally beneficial. It's a renewable, sustainable, and clean energy source. It aids in shielding the ecosystem from the effects of climate change. This energy has a longer lifespan, produces large output returns, and is also reasonably priced.
It is the process by which a substance reacts to light by producing voltage and electric current, and it can be defined with the help of the photovoltaic effect. It is related to the photoelectric effect; in both situations, light absorption causes an electron to a more energetic state. The main distinction is that, while the photoelectric effect usually uses the electron being ejected from the material, the photovoltaic effect is used when the excited charge is still held within the material.

1.3SOLAR CELL

One sort of technology that uses sunlight to create energy is solar cells. They constitute a vital part of solar panels or modules, which gather solar energy and put it to various uses, including producing electricity.The photovoltaic effect is the foundation for solar cell operation. An electric current is created when sunlight strikes the semiconductor material of a solar cell, igniting the electrons. It is possible to trap this current and use it to produce energy. Because crystalline silicon (c-Si) is low-cost, high-efficiency, and long-lasting, it is the most widely used component in solar cells.Three fundamental characteristics are needed:

1) The production of excitons or an electron-hole pair through the absorption of light.
2) The application of an internal field to assist in the opposing charge carriers' separation.
3) The autonomous extraction of the carriers to an external circuit.

1.3.1 GENERATIONS OF SOLAR CELL

Since the invention of the first solar cell in the late nineteenth century, there has been a substantial evolution in this field. This evolution may be studied by grouping solar cells into three primary categories. This classification is based on the materials and their application.

1.3.2 FIRST GENERATION

This generation of solar cells is often referred to as classic or conventional solar cells because it was the start of their evolution. More than 80% of the solar panels in use today are these ones. Polycrystalline, monocrystalline, and single III-V junction (GaAs) silicon are used in this generation of solar cells. This generation has provided the highest amount of commercial use of solar technology to date. Even though they use a proven technology and have a respectably good solar cell efficiency, their cost is a disadvantage. Because silicon requires a large amount of energy to purify, producing silicon-based solar cells is quite expensive.

1.3.3 SECOND GENERATION

The primary reason first-generation cells are so expensive is that wafer-based technology requires a significant amount of material. Tin films are therefore used as the basis for second-generation solar cells, sometimes referred to as thin film solar cells, which are made to reduce the cost factor. They are made by applying thin layers of various materials to substrates made of glass or plastic. Despite being the cheapest solar cell material to date, amorphous silicon's thinner composition results in lesser efficiency than first-generation silicon-based solar cells.
CdTe cells, with a record efficiency of 21%, are competitively priced due to their widespread availability. Furthermore, the spectrum of cadmium is larger and more similar to the sun's than that of silicon. By utilizing energy-efficient manufacturing procedures, CIGS also lowers the production's net cost. It has a lower efficiency than silicon, but it has better thermal stability. Despite the benefits of these materials, their usage is discouraged due to the high toxicity of the chemicals employed in Cd and CIGS cells. Concerns over toxicity and low efficiency made the development of third-generation solar cells possible.

1.3.4 THIRD GENERATION

This generation offers a vast array of innovative technology aimed at reducing costs and boosting production.
Among them are:

- Organic solar cells: these cells use organic semiconducting materials, Usuallypolymers, to generate energy.Although silicon-based cells are now more efficient, they have the potential to be made in large quantities at a fair cost. Dye-sensitized solar cells(DSSC):photons are absorbed by a layer of dye molecules, which then transfer the energy to a semiconductor material to generate power. Despite their limited efficiency, they are known for their aesthetic appeal and can work well in dim light. They employ perovskite as the layer that absorbs photons.
- Quantum dot solar cells (QDSCs): QDSCs use semiconductor nanoparticles, or quantum dots, that exhibit quantum confinement phenomena toenhance their light-absorption capacities. They might be very efficient and have tunable bandgaps.

1.3.5 FOURTH GENERATION

Research on fourth-generation solar cells is still ongoing. The objective is to overcome the limitations of previous iterations through the exploration of innovative concepts such as tandem structures, multi-junction solar cells, and novel materials. These technologies strive for even more efficiency, durability, and cost reductions.

Chapter 2
Literature Review

2.1 PEROVSKITE SOLAR CELL

A mixture of lead, halogens, and cesium was created later in 1892 [8]. Perovskite oxides have been reported to be suitable for use in glass and ceramic goods. Electromechanical transducers based on ferroelectric and perovskite crystalline oxides have been in use since 1955. Electrochemical cells designed to convert alcohols to ketones are used in perovskite-based cathode catalysts. PSCs are a particular kind of solar cell where the active layer that gathers light is composed of perovskite. Typically, this substance is a blend of inorganic and organic chemicals based on tin or lead halides.

2.2 BASIC STRUCTURE

The perovskite material is derived from an ABX_3 class of chemical components of perovskites. One form of organic-inorganic metal halide combination is used in the production of solar cells. In a perovskite structure, the metal cations B (Pb2+, Sn2+, Ge, etc.) and the halogen anion X (Cl-, Br-) are situated at the vertex of the face-centered cubic lattice[2]. A three-layered network structure that is stable is formed by connecting the metal-halogen octahedra.

Perovskite solar cells are typically composed of many layers that work together to absorb solar light and transform it into electrical energy. Here is a summary of the essential elements.
1. Substance: The PSC's substrate, or bottom layer, provides mechanical support and stability. Usually made of glass or a malleable substance like plastic.

2. Conductive Transparent Layer: This layer of visible conductivity, which is placed on top of the substrate, is frequently made of transparent conducting polymers or indium tin oxide (ITO). This layer lets light through while acting as an electrode to collect the generated electric current.

3. The term electron transparent layer(ETL) refers to a layer that facilitates electron movement within a cell. TiO2 and other metal oxides are commonly used as materials for the ETL in PSCs. Electrons can migrate toward the electrode with the help of the ETL, which helps to remove them from the absorbing layer.

4. Perovskite layer: It is responsible for absorbing sunlight and generating electrical charges. The perovskite layer’s superior light absorption allows photons to be simulated into holes and electrons.

5. Hole Transport Layer (HTL): This layer moves the positively charged holes made in the absorber layer. Polymers or organic small molecules are common materials used in the HTL. The HTL helps as the holes are gathered and directed towardsthe electrode.

6. Contact/Counter Electrode: located about HTL, a contact electrode is usually composed of metals such as gold, silver, or carbon-based compounds. By collecting the holes made in the perovskite layer, these electrodes complete the electric circuit.

2.2.1PLANE HETEROSTRUCTURE

Since there is no mesoporous metal oxide, the entire structure is straightforward.The light-absorbing perovskite layer is placed between the HTL and the ETL. The efficiency of this kind of solar cell can be adjusted by changing the characteristics of the contact between its several PSC layers. Its disadvantage is that it exhibits current density, also known as open-circuit voltage hysteresis, in addition to its regulated efficiency.

2.2.2PEROVSKITE LIGHT-ABSORBING LAYER

Light absorption and photoelectric conversion are two perovskite solar cell components that are reliant on the perovskite materials. "Simple perovskites" are perovskite compositions where the A-, B-, and X-sites are all occupied by a single ion. One of the key elements in raising photoelectric conversion efficiency is the development of materials and architecture.

2.2.3 ELECTRON TRANSPORT LAYER

The main objectives of ETL are to collect the electrons generated by photons striking the layer and, in order to prevent electron-hole recombination, to stop the holes from traveling in the direction of the counter electrode.

2.2.4HOLE TRANSPORT LAYER

Similar to ETL, HTL captures charge carriers but additionally accumulates holes and prevents electron-hole recombination. In order for perovskite materials' valence band to function as a hole transport route, the material's most occupied molecular orbital (HOMO) compatibility is required. PSCs use organic and inorganic materials as hole transporters.

2.3 PROPERTIES OF PSC

PSCs have attracted a lot of interest lately as a potential component for solar systems that are both affordable and efficient. Their wide range of component parts, low manufacturing temperature, tunable band gap, and They are superior to the majority of thin film absorber

materials in a number of areas thanks to their high absorption coefficient. In particular, PSC device hysteresis is greatly influenced by the dielectric constant. The modeling findings show that the degree of hysteresis can be decreased with a low dielectric constant ETL.

2.4 WORKING

The PSC acts as a result of the active absorber perovskite layer functioning as an intrinsic semiconductor layer, the hole-transporting layer functioning as the P+ layer, the electron-transporting layer functioning as the N+ layer, and so on…like a pin diode.Electrodes for electrical access are provided by the access are provided by the metallization layers. The integrated field is received by the I-layer. When the device is turned on, the photons the I-layer and create electron-hole pairs there. Eventually, they settle onto the appropriate electrode.

Chapter 3

Simulation and Methodology

3.1 SCAPS-1D Solar Cell Simulation Software

An overview of SCAPS-1D, a well-liked program for modeling solar cells, is given in this section. It explains how it can model and simulate several aspects of solar cells, including their electrical and optical characteristics,carrier transport, and recombination process. The significance of simulation software in solar cell research is also emphasized in this area. It enables researchers to optimize device performance and learn more about the physics at play. A simulation tool called SCAPS-1D was created expressly to study and simulate solar system performance. It offers a framework for evaluating and improving the electrical and optical characteristics of many kinds of photovoltaics, such as but not limited to thin-film, perovskite and silicon-based solar cells. This is a summary of the functions, applications, underlying codes, and concepts of SCAPS-1D:

3.1.1WORKING PRINCIPLE

SCAPS-1D simulates solar cell dynamics through the use of numerical methods**.** It uses a one-dimensional modeling framework, taking into account the layers that make up the device construction along the thickness direction. By resolving a series of links using differential equations, SCAPS-1D computes and forecasts several parameters, including Q.E., carrier density profiles, J-V characteristics, and electric fields inside the solar cell structure.

3.1.2 USES OF SCAPS-1D:

1. Device Design and Optimization: To maximize the performance of solar cells, researchers and engineers can investigate various device topologies, layer materials, and parameters using SCAPS-1D. It supports the design process by forecasting how different modifications will affect the electrical output and assisting in the identification of efficiency-boosting tactics.

2. Parameter extraction: With the software, users can extract and calculate vital characteristics of materials and devices, including mobility values, interface recombination velocities, carrier lifetimes, and trap densities. These retrieved characteristics can provide useful details on the quality of the material and the interfaces inside the structure of the solar cell.

3. Sensitivity Analysis: With the aid of SCAPS-1D users can assess howchanges in material qualities, layer thicknesses, and other factors affect the functionality of the device. This approach directs experimental efforts and helps discover crucial parameters that have a major impact on solar cell efficiency.

3.1.3 UNDERLYING CODES AND CONCEPTS

Physical theories and mathematicalequations that explain solar cell behavior are the basics of SCAPS-1D. To solve these equations and replicate the functioning of the gadget, the program makes use of numerical techniques and iterative algorithms. The following are few of the fundamental ideas and codes utilized in SCAPS-1D:

1. Drift-Diffusion Equations: Drift-Diffusion which includes charge carrier transport mechanismssuch as diffusion caused by gradients in carrier concentration and drift caused by electric fields, is used by SCAPS-1D. the flow of electrons and holes within the structure of a solar cell is described by these equations.

2. Shockley-Read-Hall Recombination (SRH):The SRH model takes charge carrier recombination at material defect locations into account. The methods in SCAPS-1D are designed to compute and take into account the effect of SRH recombination on device performance.

3. Optical modeling:SCAPS-1D takes into account light transmission and absorption inside the solar cell structure. To account for light absorption in various layers and interfaces, it makes use of ideas like Lambert-Beer's law and takes into consideration the wavelength-dependent optical characteristics of materials

4. Interface and Contact Models: To account for phenomena like surface recombination and tunneling, the software provides models to characterize the electrical behavior and recombination qualities at material interfaces and contacts.

5. Fitting Procedures and Optimization Algorithms for Comparing Simulation and Experimental Results: SCAPS-1D integrates these techniques. This makes it possible to identify precise material and device parameters that most closely resemble the feature of the measured device.

In general, SCAPS-1D simulates and analyzes photovoltaic performance using a combination of numerical techniques, physics -basedmodels, and optimization algorithms. SCAPS-1D advances solar cell technology by offering a comprehensive platform for device design, optimization, and parameter extraction. This platform also helps researchers and engineers discover new ways to improve the efficiency of solar energy conversion.

3.1.4 NUMERICAL METHODS USED IN SCAPS-1D: -

The electrical and optical equations for the photovoltaic device simulation in SCAPS-1D are solved numerically using the Transfer Matrix Method (TMM). By taking into account the transmission and reflection of light at each interface inside the structure, the TMM is an effective method for modeling multi-layered systems. The TMM used in SCAPS-1D enables the computation of optical characteristics including absorption and transmission coefficients in addition to the tracking of light as it moves through the different layers of the solar cell. This data is essential for precisely simulating photon absorption and computing the device's Q.E.

SCAPS-1D uses other numerical techniques in addition to the TMM to solve the drift-diffusion equations, which explain carrier movement and recombination inside the solar cell structure. These techniques usually entail solving a set of coupled differential equations that come from discretizing the device structure into a set of computational points or nodes along the thickness direction.

Although the specifies of the code implementation used in SCAPS-1D are not publicly available, it is expected to solve the drift-diffusion equations using well-known numerical algorithms like the finite difference or finite element methods. By employing discrete differences to approximate the derivatives in the equations, these approaches solve the resulting equations iteratively, yielding carrier profiles and devices properties.

It's crucial to remember that SCAPS-1D is a private software tool, and that the particulars of its implementation—such as the selection of its coding schemes and algorithms—are not accessible to the general public. In order to simulate solar cell system with efficiency and accuracy, the underlying numerical algorithms and codes utilized in SCAPS-1D were probably enhanced. This means that researchers and engineers have a solid platform on which to conduct their investigations and optimizations.

3.2 wxAMPS

The original AMPS algorithm serves as the foundation for wxAMPS, a simulation program for solar cells that has been developed lately.[1] The GUI of wxAMPS enables quick data entry and enhanced results presentation for analysis and comparison with the aid of the cross-platform C++ toolkit wxWidgets. The program borrows its fundamental physical concepts from AMPS [2]. The wxAMPS algorithm has improved convergence and stability by integrating the newton and Gummel techniques. Shunt and series resistance effects that have nothing to do with the main diode are also included.

These can be made from a variety of materials, including thin films of CdTe and CIGS, as well as crystalline and amorphous Si materials.The most recent version is available for use on the WIKI website.

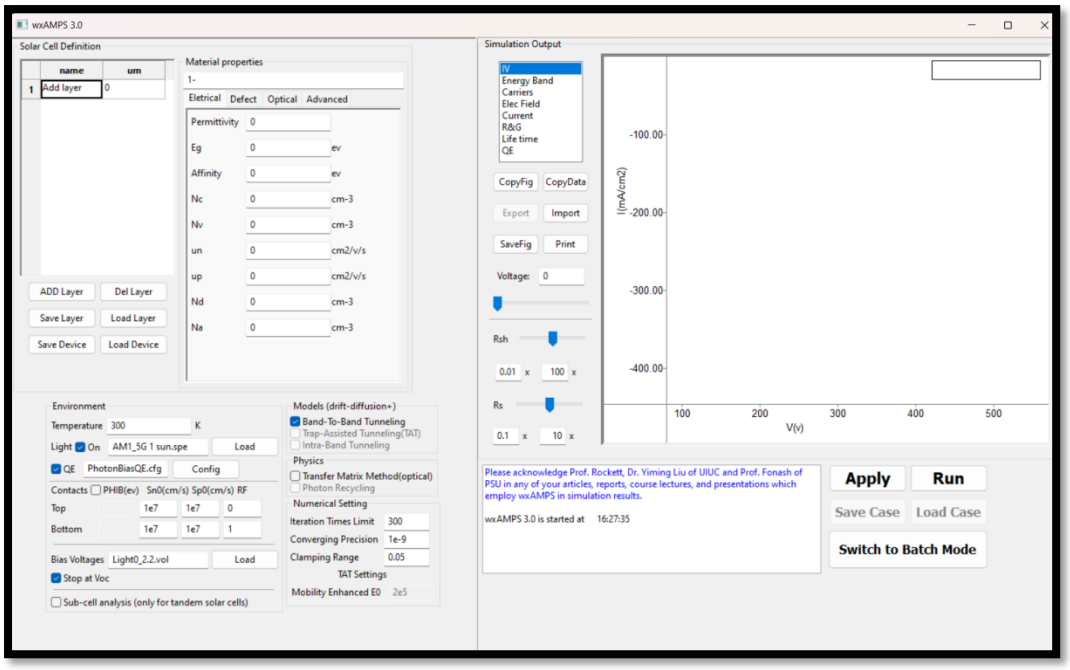

Fig 1. wxAMPS software interface.

3.3 $KSnI_3$ OPTIMIZATION

A simulation model for lead-less $KSnI_3$ perovskite solar cells was set in wxAMPS to study different device parameters. It has a bandgap of 1.84 eV with 10.4 permittivity and other required properties listed in Table 1. FTO/ETL/$KSnI_3$/HTL/W device structure is used for the study of $KSnI_3$-based PSC. Various ETLs such as ZnSe and WS_2 along with multiple HTLs such as CBTS, PEDOT: PSS, Cu_2O, and CdTe were analyzed.

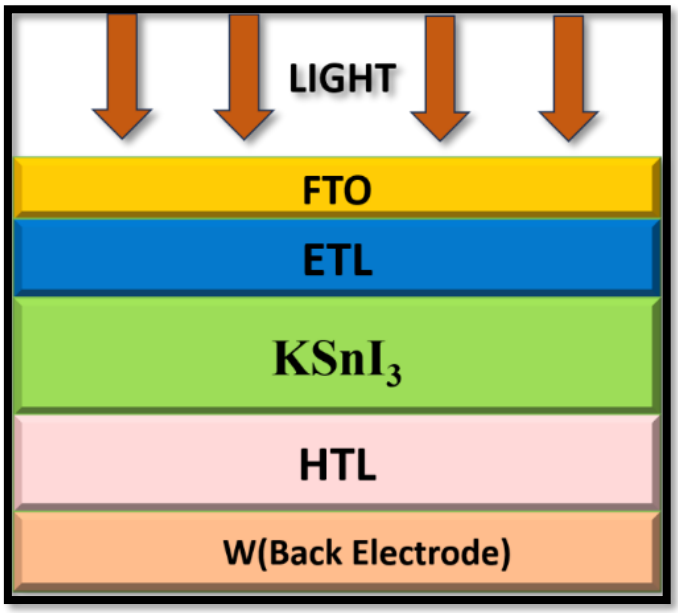

Fig 2. Device structure of PSC.

Table 1. Different properties of various HTL's.

Parameters	CBTS	Cu_2O	PEDOT:PSS	CdTe
Thickness (nm)	100	50	50	50
E_g (eV)	1.9	2.2	1.6	1.5
χ (eV)	3.6	3.4	3.4	3.9
$\varepsilon/\varepsilon_o$	5.4	7.5	3	9.4
N_C (cm^{-3})	2.2×10^{18}	2×10^{19}	2.2×10^{18}	8×10^{17}
N_V (cm^{-3})	1.8×10^{19}	1×10^{19}	1.8×10^{19}	1.8×10^{19}
μ_e ($cm^2V^{-1}S^{-1}$)	30	200	4.5×10^{-2}	3.2×10^{2}
μ_h ($cm^2V^{-1}S^{-1}$)	10	8600	4.5×10^{-2}	40
N_D (cm^{-3})	-	-	-	-
N_A (cm^{-3})	1×10^{18}	1×10^{18}	1×10^{18}	2×10^{14}
Reference	[3-4],[6]	[4]	[3],[4]	[23]

Table 2. Different properties of ETL's.

Parameters	**WS_2**	**ZnSe**
Thickness (nm)	100	100
E_g (eV)	1.8	2.81
χ (eV)	3.95	4.09
$\varepsilon/\varepsilon_o$	13.6	8.6
N_C (cm^{-3})	1×10^{18}	2.2×10^{18}
N_V (cm^{-3})	2.4×10^{19}	1.8×10^{18}
μ_e ($cm^2V^{-1}S^{-1}$)	100	400
μ_h ($cm^2V^{-1}S^{-1}$)	100	110
N_D (cm^{-3})	1×10^{18}	1×10^{15}
N_A (cm^{-3})	-	-
Reference	[4]	[3],[10]

Table 3. Various Parameters of PSC layers.

Parameters	**Cu_2O**	**$KSnI_3$**	**WS_2**	**FTO**
Thickness (nm)	50	300	100	100
E_g (eV)	2.2	1.84	1.8	3.5
χ (eV)	3.4	3.44	3.95	4.5
$\varepsilon/\varepsilon_o$	7.5	10.4	13.6	9
N_C (cm^{-3})	2×10^{19}	2.2×10^{18}	1×10^{18}	2.2×10^{18}
N_V (cm^{-3})	1×10^{19}	1.8×10^{19}	2.4×10^{19}	1×10^{19}
μ_e ($cm^2V^{-1}S^{-1}$)	200	21.28	100	2×10^3
μ_h ($cm^2V^{-1}S^{-1}$)	8600	19.46	100	2×10^3
N_D (cm^{-3})	-	1×10^{15}	1×10^{18}	2×10^{19}
N_A (cm^{-3})	1×10^{18}	1×10^{15}	-	-
Reference	[4]	[1] ,[2]	[4]	[3],[8]

Chapter 4

Results and Discussion

4.1 $KSnI_3$SIMULATION

A simulation model for lead-less $KSnI_3$ perovskite solar cells was set in wxAMPS to study different device parameters. Various ETLs such as ZnSe and WS_2 along with multiple HTLs such as CBTS, PEDOT: PSS, Cu_2O, and CdTe were analyzed.

4.1.1 DIVERSIFICATION OF ETL AND HTL

Charge carriers in the solar cell are transferred by the ETL and HTL. Although the HTL makes it easier to transmit holes. ETL helps electrons to move in the external circuit, to minimize charge recombination and maximize electrical current generation, which improves overall solar efficiency, effective transport is crucial. We have explored two ETLs (WS_2 and ZnSe) and four HTLs (Cu_2O, CBTS, CdTe, PEDOT: PSS). These particular HTLs and ETLs were chosen due to their positive performance results, which have been reported in previous research, whereby they showed a significant increase in PCE and favorable properties that made them suitable for integration into solar cell designs. Quantum efficiency's reduction is possibly accounted for by decreased at longer wavelengths and near-surface recombination [3].

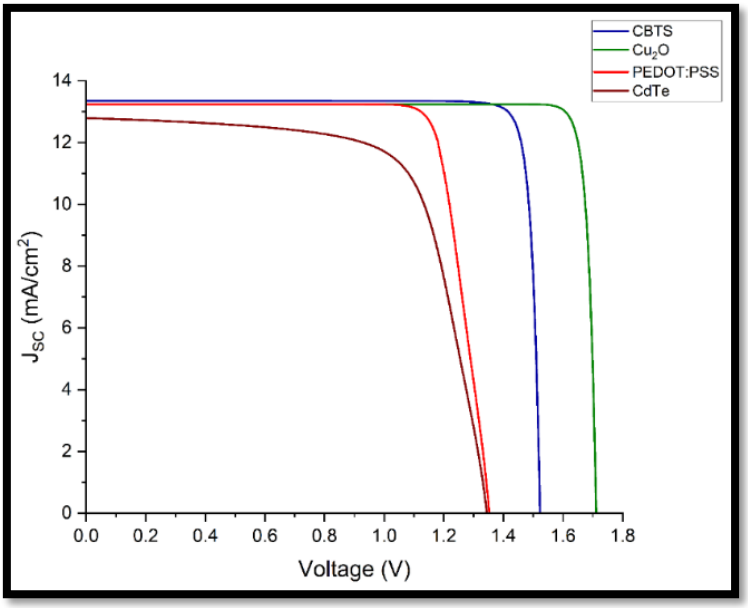

Fig.3. JV characteristic graph for WS_2 (ETL) with multiple HTL.

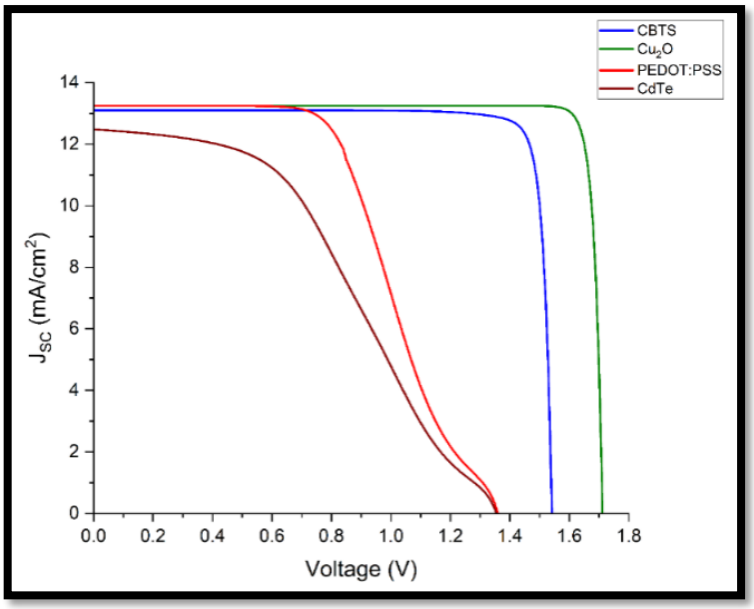

Fig.4. JV characteristics graph for ZnSe (ETL) and multiple HTLs.

4.1.2 CHANGING THICKNESS OF $KSnI_3$ LAYER

In wxAMPS, the thickness of absorber layer is varied and characteristics of the $KSnI_3$ SC was examined. It was changed from 100 nm with interval of 100. The above tables indicate other parameters related to the absorber layers, FTO, HTL and ETL were maintained constant. It was observed that efficiency rose together with thickness because photons could not sufficiently absorb light at lower thickness. Recombination of carriers happen for thick film, hence it started to decrease after 800 nm. A maximum of 24.88% efficiency was observed at 730 nm. Fill Factor (FF) values remain constant at 94.82% from 100 nm to 1000 nm. With an increase in thickness, current density value increases, from 11.74 to 13.30 mA/cm^2. Thickness of the active layer plays a vital role in optimizing the PCE of solar cells. It should be chosen appropriately to maximize J_{SC}. In larger absorber layers, the recombination of electrons and holes is affected by electric field, leading to a decrease in efficiency. Because of increased internal power dissipation and series resistance in thick absorbing layers, FF has an inverse relationship with absorber thickness [3]. The graphical presentation depicts the change in PCE, FF, V_{OC}, J_{SC} in Fig.5.

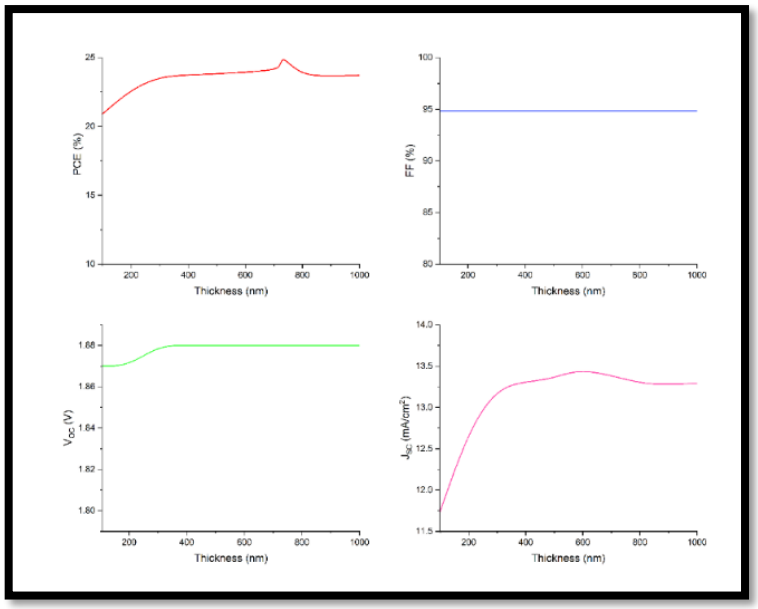

Fig.5. Variation of thickness affecting different parameters.

4.1.3 VARIATION OF TEMPERATURE

The impact of temperature on PSC parameters is examined and we have varied it from 200 to 800 K. We saw a decline in PCE, FF and V_{OC}. At 200 K, the maximum efficiency of 23.62% is computed and at 800 K, the minimum efficiency of 8.19%. As temperature rises, FF declines. At 200 K, it reaches a maximum value of 94.82% and at 800 K, it drops to 73.09%. The temperature has a huge impact on how well the SC works. Usually, solar panels operate above 300 K. Raising the temperature is said to increase strain and stress on structures. Many parameters like carrier concentration, PSC's efficiency are affected by increased temperature. A little increase in J_{SC} is also brought about by temperature increases, this is due to the lesser energy band gap, more electron-hole pairs are created. An increase in series resistance, a decrease in carrier diffusion length and the creation of additional interfacial defects could account for the decrease in V_{OC} as temperature increases [15].

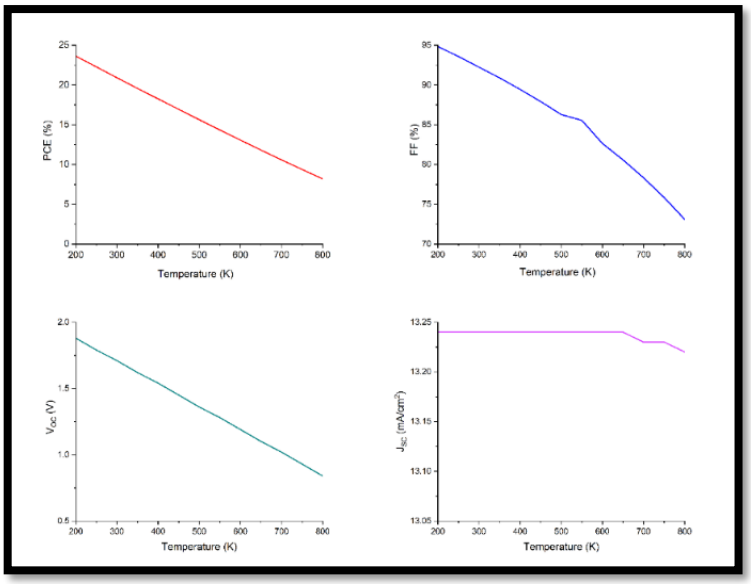

Fig. 6. Variation of temperature affecting different parameters.

4.1.4 VARIATION OF ELECTRON AFFINITY

The electron affinity is varied from 3.4 eV to 4.6 eV while maintaining the same properties for the other layers with the configuration FTO/ZnSe/$KSnI_3$/Cu_2O/W. Using the "Origin pro2024" software, we gathered and plotted the data and examined the solar cell properties. An efficiency of 21.40% is observed at the optimal value of electron affinity of 4.4 eV. With minor and steady variations in these parameters, the graphical analysis demonstrates other parameters exhibit stability.

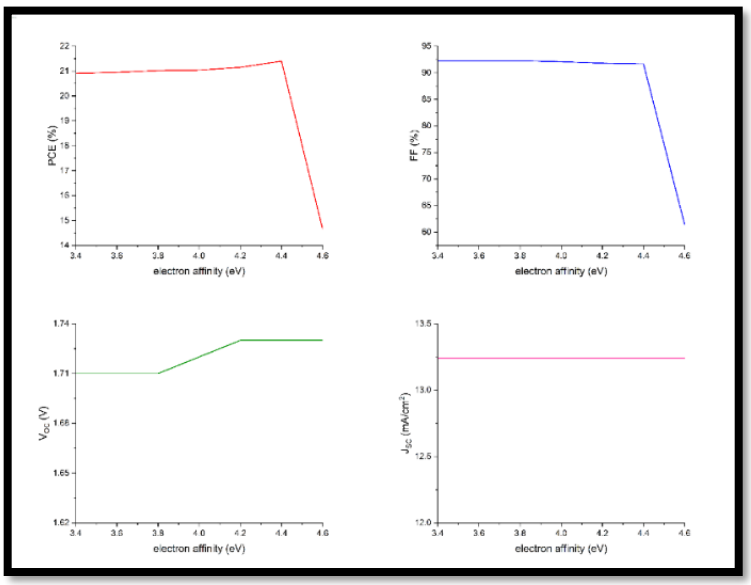

Fig.7. Variation of electron affinity affecting different parameters.

4.2 COMPARISON WITH SCAPS-1D RESULTS

The simulation results of SCAPS-1D software are used to validate the results of wxAMPS. To determine the differences in JV characteristics between the devices, the two software programs ran simulations of $KSnI_3$ with absorber thickness, permittivity set to 300 nm and 3.44 eV respectively. All of the simulations using SCAPS-1D were conducted at temperature of 300 K, just like wxAMPS simulations. Table 4 depicts the comparison of the software simulation results from wxAMPS and SCAPS-1D. These kinds of results were quite similar to earlier researches and the variation in outcomes between the two simulation techniques were satisfactory.

Table 4. Various PSC layers and their results.

Device Structure	FF(%)		V_{OC} (V)		J_{SC} (mA/cm^2)		PCE (%)	
	SCAPS-1D	wxAMPS	SCAPS-1D	wxAMPS	SCAPS-1D	wxAMPS	SCAPS-1D	wxAMPS
FTO/ZnSe/$KSnI_3$/CdTe/W	36.37	42.07	1.31	1.35	13.12	12.48	6.27	7.11
FTO/ZnSe/$KSnI_3$/Cu_2O/W	89.30	92.23	1.41	1.71	14.47	13.20	19.44	20.91
FTO/ZnSe/$KSnI_3$/CBTS/W	74.72	89.18	1.40	1.54	14.84	13.10	15.61	18.01
FTO/ZnSe/$KSnI_3$/PEDOT:PSS/W	50.57	55.52	1.32	1.36	14.52	13.24	9.72	10.00
FTO/WS_2/$KSnI_3$/CdTe/W	70.47	69.37	1.33	1.34	14.95	12.79	14.07	11.93
FTO/WS_2/$KSnI_3$/Cu_2O/W	86.64	92.24	1.41	1.71	15.16	13.24	18.54	20.91
FTO/WS_2/$KSnI_3$/CBTS/W	86.40	90.48	1.40	1.52	15.59	13.35	18.99	18.40
FTO/WS_2/KSnI3/PEDOT:PSS/W	77.66	81.78	1.34	1.35	15.88	13.24	16.55	14.65

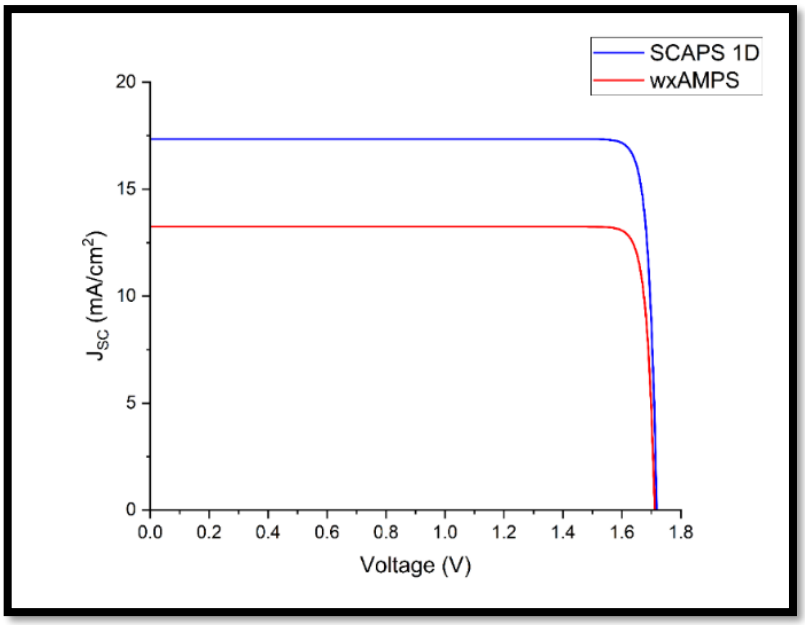

Fig.8. Graph showing JV characteristics of FTO/ZnSe/$KSnI_3$/Cu_2O/W.

Chapter 5

Conclusion

As a result, we may conclude that $KSnI_3$ is a promising alternative for non-leaded PSCs and has fruitful application. The device performance was examined by varying the ETLs and HTLs. As we increase the thickness, PCE also increases and we get maximum PCE of 24.88 % at absorber layer thickness of 730 nm. We get best efficiency for Cu_2O as HTL and ZnSe as ETL by using wxAMPS software. Finally, the device structure FTO/ZnSe/$KSnI_3$/Cu_2O/W with optimum efficiency of 24.88% was best suited for solar applications. This work unequivocally shows that, in order to expand on the understanding gained from the simulation-based results reported here, more research on $KSnI_3$ based PSC is required. This research should especially focus on actual experimentation, various optimum parameters proposed in this research, may be used in practical investigations in the future.

APPENDICES

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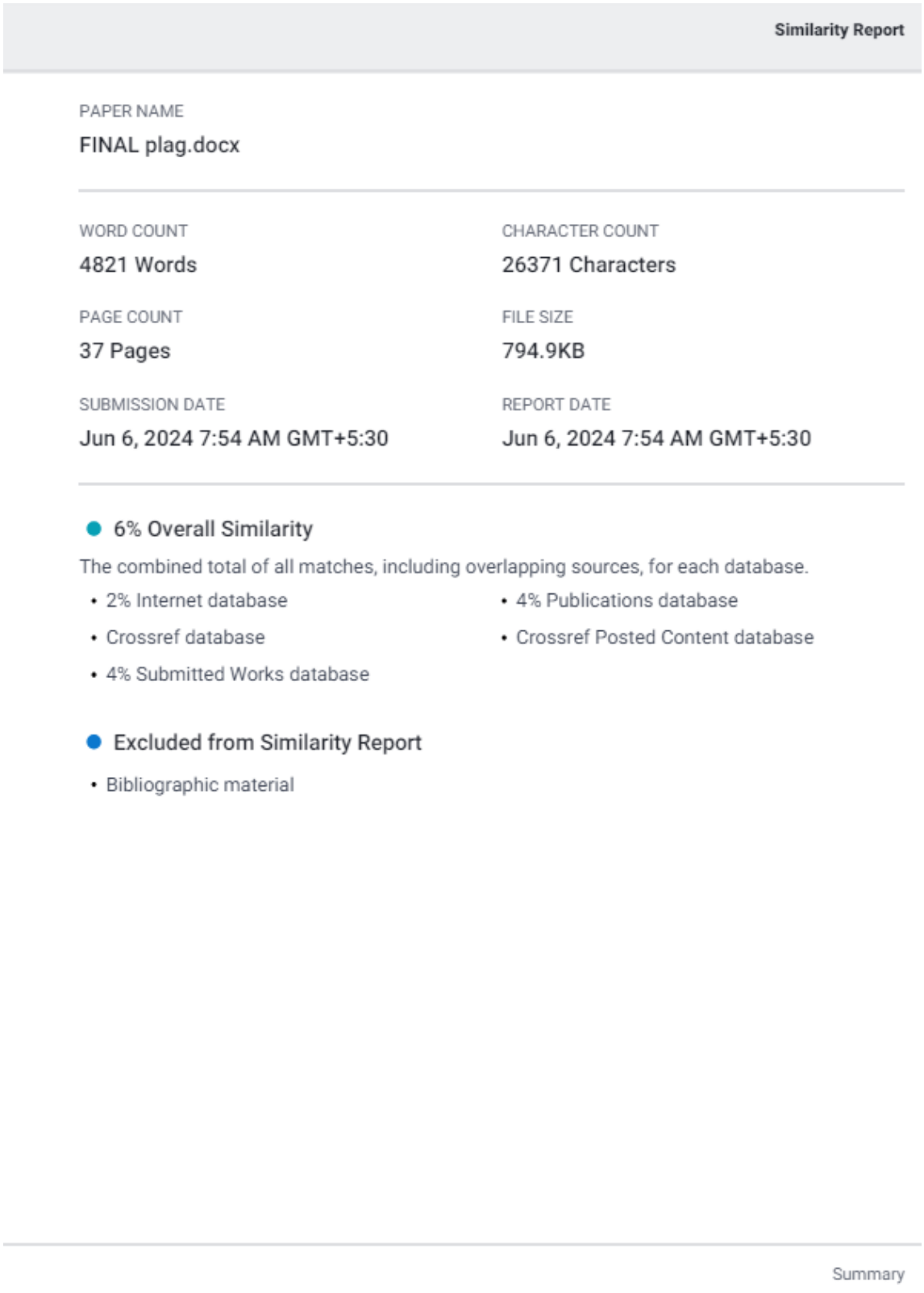

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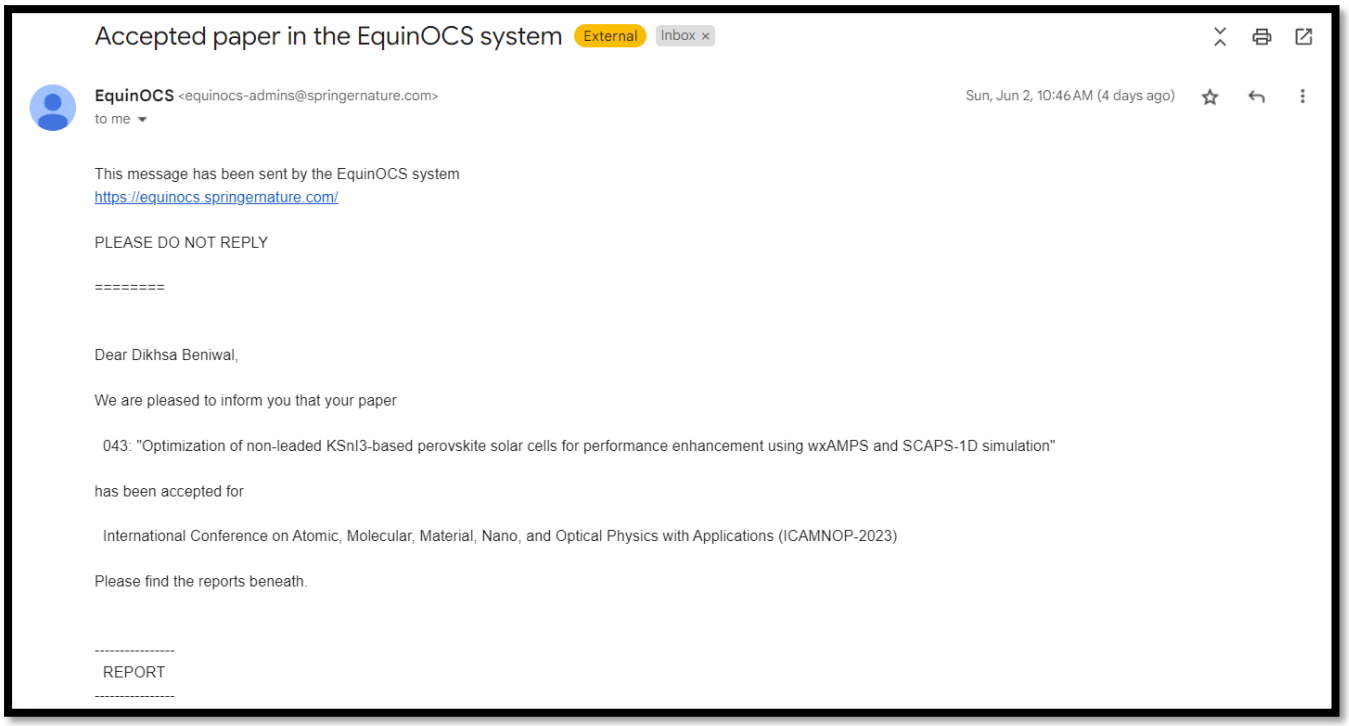

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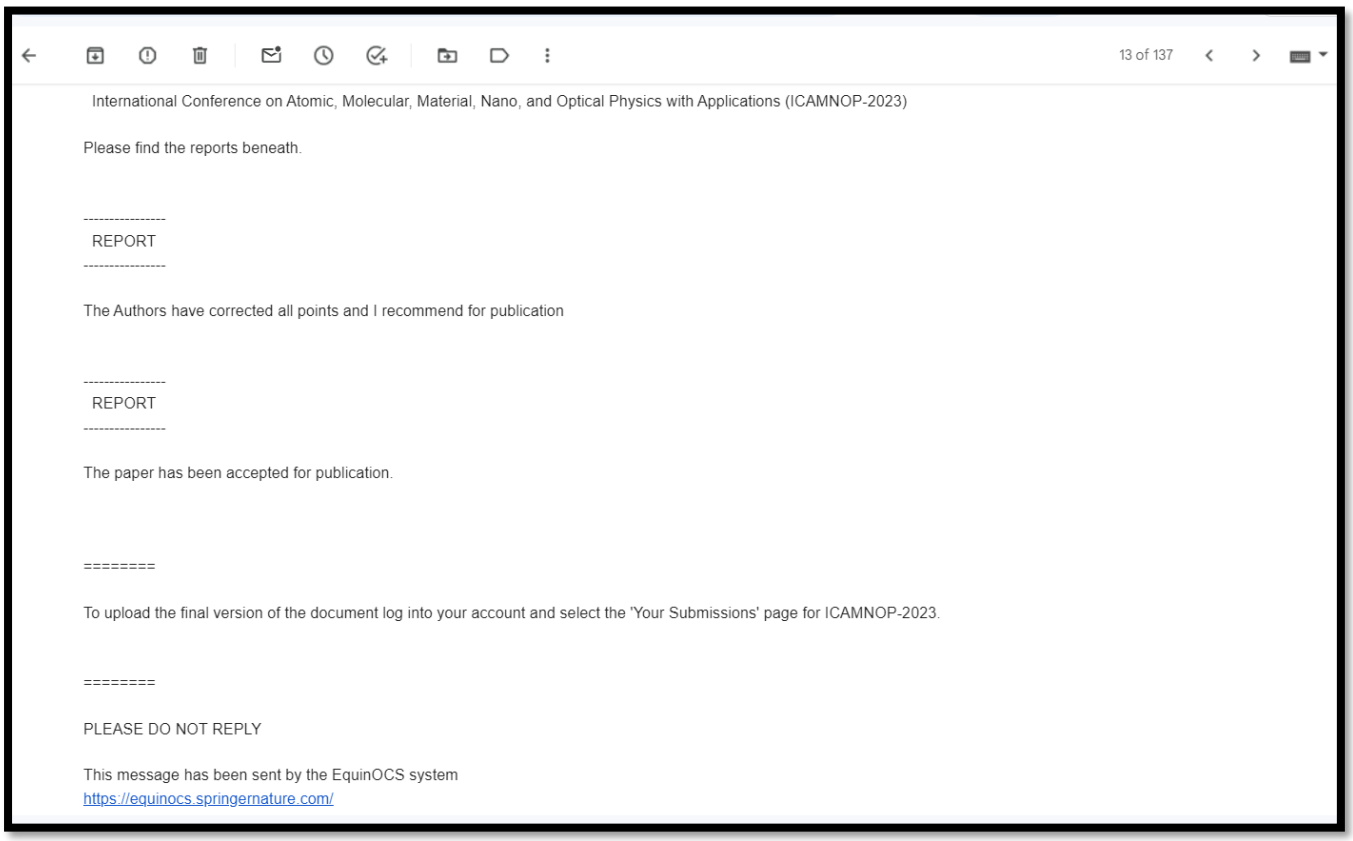

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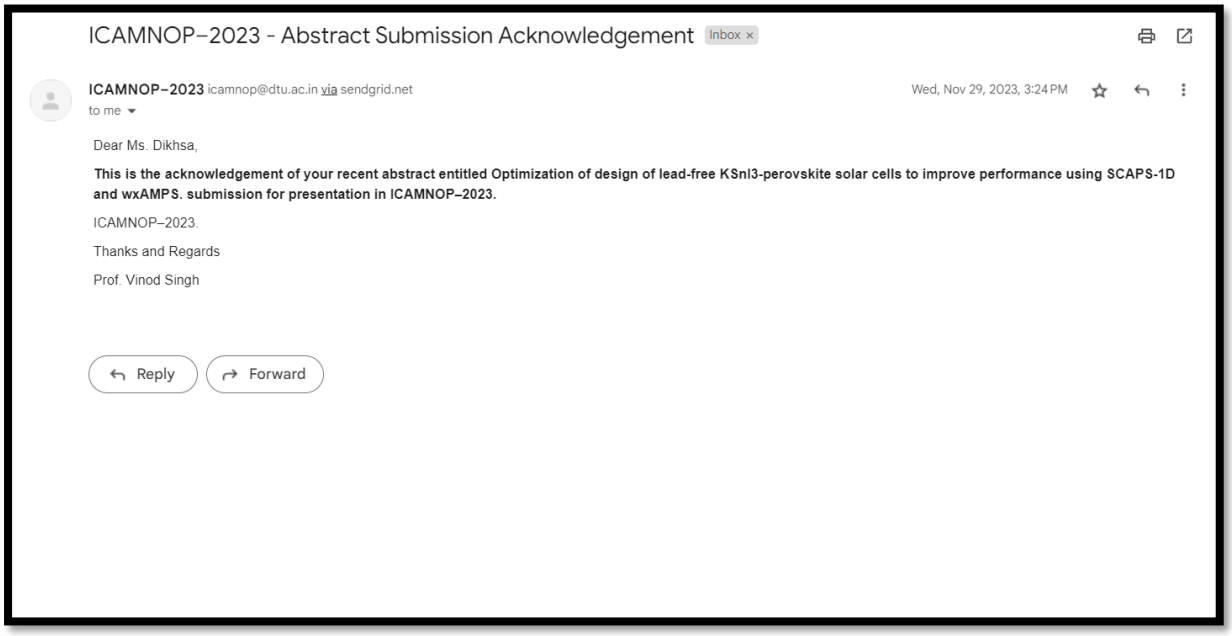

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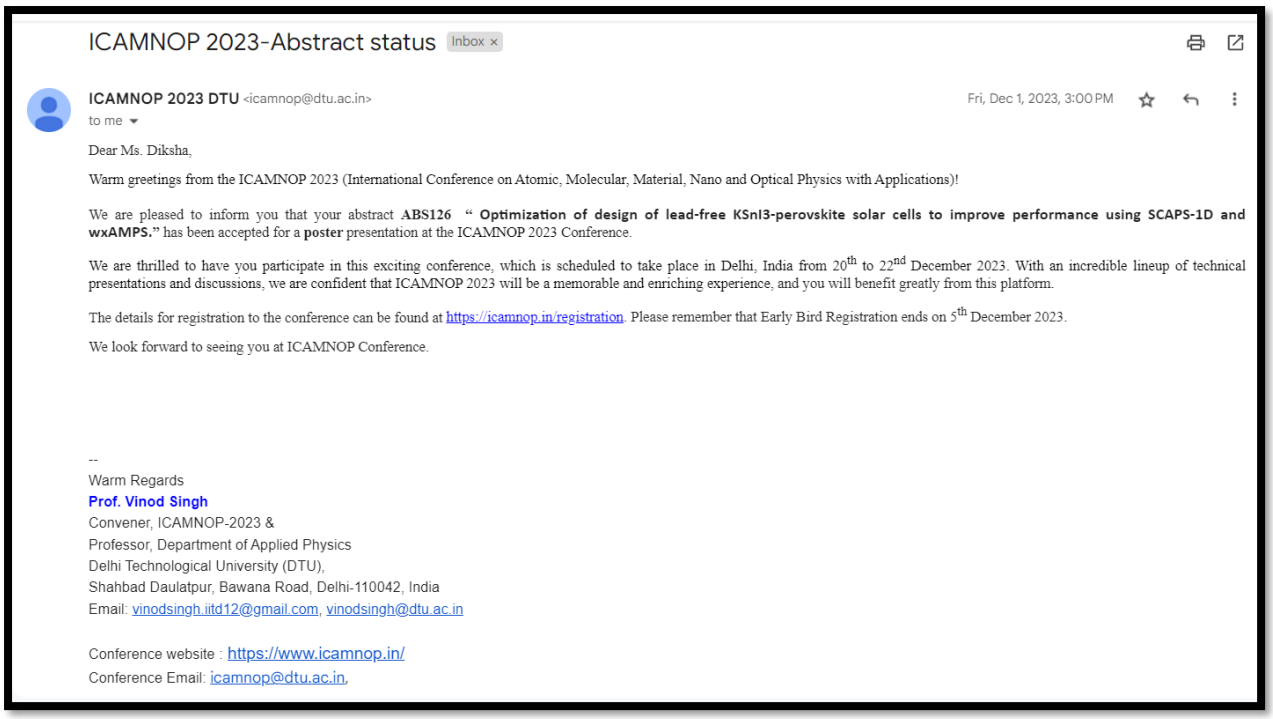

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Warm Regards
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Convener, ICAMNOP-2023 &
Professor, Department of Applied Physics
Delhi Technological University (DTU),
Shahbad Daulatpur, Bawana Road, Delhi-110042, India
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