



THE EFFECT AND PERFORMANCE OF ELECTRON TRANSPORT MATERIAL ON C60-BASED PEROVSKITE SOLAR CELL

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ABSTRACT

Solar Energy System explored the use of photovoltaic technology in converting solar irradiance using the required materials but effective materials are required in the conversion process at different segment of solar cells. Electron Transport Material (ETM) plays a remarkable role in the conversion of irradiance received from the sun into electricity. This work presents the behaviours of ETM such as fullmade (C60) with respect to organic Hole Transport Material (HTM) NiO and an inorganic perovskite material called potassium germanium chloride (K_3GeCl_3) as an absorber in the solar cell. Using finite element method as contain in COMSOL Multiphysics software, Poisson and electrical transport equations were computed for an optimal solution with the highest output conversion efficiency of the solar cell, the thickness size of the electron transport layer and light absorption layer. A specific designed structure with an architectural position of FTO/C60/ K_3GeCl_3 /NiO/Au was used for the purpose of this investigation. This designed structure was able harness a power conversion efficiency (PCE) of 19.04% with an output open circuit voltage of 0.78V, a short circuit current of 31.02mA, and fill factor of 0.787. The results show that effective material in the ETM and HTM can be used to assist in creating an improved, efficient and good performance perovskite based solar cell.

1.0 INTRODUCTION

Solar Photovoltaic technology is one of the major drivers towards sustainable energy globally. Solar photovoltaic systems have since became the most widely and commonly used renewable energy technology in both rural and urban areas around the world, and this have been particularly for both commercial and residential buildings. The demand for energy around the world is directly proportional to the population increased more especially in the sub-Saharan Africa (SSA) as indicated in (IRENA and AfDB, 2022). The use of solar energy has emerged significant and most viable option for solution due to the energy needs in both commercial and residential buildings (Vural, November 2019). Abundant radiation is some part of the world have made solar energy an energy demand solution for the requirement of the various loads. But this abundant energy that is left untapped can only harness using the right technology, the right materials and optimisations tools (IRENA 2024). Perovskite solar cell is among the most

promising, emerging solar cells technologies and the fourth-generation solar cells that utilizes organic-inorganic perovskite materials (Khalid et al., 2021). These materials have shown a significant increase in efficiency, rising from 3.8% to 25.5% in just within a decade (Perovskite et al, 2022). The aim of this study is to investigate the effectiveness of ETM and optimizing the efficiency of solar cells using diverse materials while utilising potassium germanide chloride (K_3GeCl_3) as absorber layer.

2.0 METHODOLOGY

In modelling 3D solar cell, three axes of the geometry must define unlike 2D where only axes are being considered. In 3D, x, y and z axes considered with relevant dimensions as indicated in table of parameters (Table 1). According to the settings in COMSOL Multiphysics software, the axes are being assigned as width, depth and height, where the height is the z-axis, width is the x-axis and depth is the y-axis. The geometrical input parameters values for the ETL/Absorber/HTL are as indicated Table 2, under global definition in the model builder. The geometry is classified or sub-divided based on type and material to be used in the numerical modelling. Geometrically, all the layers or regions contains different dimensions with their respective doping concentrations, which is determined by the type of layer or region. The doping concentration range from a minimum to maximum concentration as mentioned in (Belarbi et al, 2022). The COMSOL Multiphysics software uses the Finite Element Method (FEM) to solve continuity equations as shown in Equation (1) while simulating solar cells to find the current density distribution (Baig et al, 2014).

$$-\nabla \cdot (\sigma \nabla V - j) = Q \quad (1)$$

Where:

- V is the electric potential,
- j is the current density,
- Q is the generated current, and
- σ is the conductivity of the material

The semiconductor module contains all the necessary partial differential equations (PDE) which govern the electronic transportation mechanism in the semiconductor material (Rupa et al, 2023). The generation rate contributes in terms of reflecting the absorption behaviours, which added to the built-in of the current densities output in form user-defined generation while the recombination techniques are being considered within the Shockley-Read-Hall (SRH) under the trap assisted recombination (Boubakri et al, 2021).

The photo-generation rate can be expressed as.

$$G(x) = \int_0^\alpha \alpha(\lambda) \phi(\lambda) \exp(-\alpha(\lambda) x) d\lambda \quad (2)$$

where x – The depth into the solar cell from the surface

λ – The wavelength

$\alpha(\lambda)$ – The Absorption coefficient

$$\alpha(\lambda) = \frac{4\pi}{\lambda} K(\lambda) \quad (3)$$

where $K(\lambda)$ – The extinction coefficient

$\phi(\lambda)$ – The incident photons flux, as in:

$$\phi(\lambda) = \frac{\lambda}{hc} F(\lambda) \quad (4)$$

$F(\lambda)$ – The spectral irradiance, at approximated value of AM 1.5 Spectrum (Boubakri et al, 2021). Meshing also contributes significantly in determining the output of the numerical simulation, where ranges of discretisation which depend on the type of selected mesh (Zandi et al, 2020). The smaller the discretisation of the geometry the higher the degree of freedom and this degree of freedom is being generated as a result of the meshing (Parasuraman et al, 2024). The mesh ranges from extremely coarser (bigger in size) to extremely fine (smaller in size). Personal Computer (PC) or laptop need a high specification capacity to carry execute finer to extremely finer mesh due to high memory space required during the execution of the simulation (Lawal et al, 2024).

Perovskite Solar cells (PSC) is an emerging solar cell technology that has gained research attention within the last two decades with tremendous improvement in terms of power conversion efficiency (PCE) (Roose et al, 2022). Perovskite solar cells were utilized in this research to have an optimal characteristics output that can compete with the best performing solar cells that have been published. The PSC materials to be considered in this work as electron transport materials (ETM) is fullerene (C60) while NiO was considered as hole transport materials (HTM). The main absorption material based on its high absorption capacity as compared to other materials is potassium germinate chloride (KGeCl₃) (Sarhani et al, 2023).

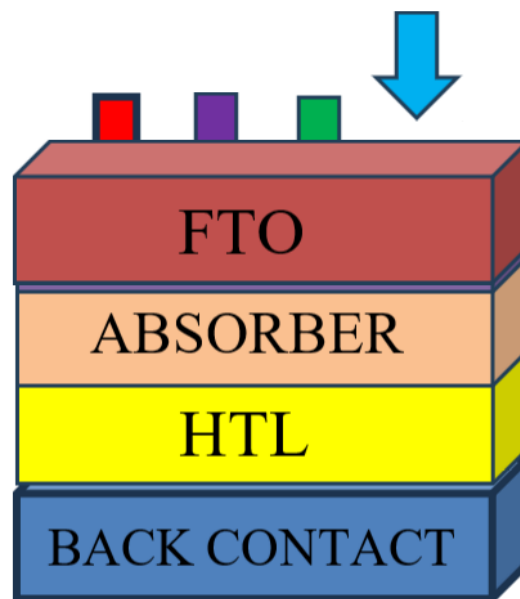


Figure 1. Typical Perovskite Solar Cell Structure (Lawal et al, 2024)

KGeCl₃ have ability to increase its charge carrier mobility and reduced recombination losses with high stability in its designed. Another absorption material used in this research is silicon material as the main substrate in the solar cells because of efficient, stability and withstand harsh environmental conditions, a metal contact is being used at both the front and the back contact as shown in Figure 1.

Table 1. General 3D Solar Cell Input Parameters Settings

Parameter	Expression	Value	Description
Temperature	300[K]	300 K	Input temperature
Voltage	0[V]	0 V	Biassing Voltage
Lambda0	300[nm]	3E-7m	Initial wavelength
Lambda1	1000[nm]	1E-6m	Final wavelength
Frequency	c_const/lambda0	9.9931E14 1/s	Initial Frequency
Width	0.2[um]	2E-7m	Width of the geometry
Depth	0.3[um]	3E-7m	Depth of the geometry
Height	0.93[um]	93E-7M	Height of the geometry
Irradiance	1000 (AM1.5)	1000Watt/m ²	Input Irradiance

Table 2. Input parameters settings for ETL/Absorber/HTL

Name	NiO	C60	KGeCl3
Thickness (um)	0.2	0.1	0.3
Band gap, E _g (eV)	3.2	1.7	1.49
Electron Affinity, χ (eV)	3.9	3.9	3.8
Relative permittivity, ϵ_r	9	4.2	7
CB effective density of states, N _c (cm ⁻³)	1e21	8e19	3.76e19
VB effective density of states, N _v (cm ⁻³)	2e20	8e19	2.10e18
Electron mobility, μ_n (cm ² /Vs)	0.02	8e-2	850
Hole mobility, μ_p (cm ² /Vs)	2	3.5e-3	450
Uniform acceptor density, N _a (cm ⁻³)	0	1e17	1e15
Uniform donor density, N _d (cm ⁻³)	5.1e19	0	1e9

3.0 Simulation Process

The simulation processes are based on the COMSOL Multiphysics numerical modelling procedures which provide the necessary information about the physical parameters of the materials used and their respective impact on the output characteristics of the semiconductor devices (Lawal et al, 2025).

4.0 RESULTS

The perovskite solar cell (PSC) structure is designed to be used in the simulation as depicted in figure 1 showing the proposed architecture. The physical parameters of the PSC materials are contained in Table 1. In carrying out this simulation a constant input irradiance of 1000Wm² as found at AM1.5G at a temperature of 300K. Also, thermal velocities of 10⁷ cm^{-s} are granted to both the electron and hole while Shallow uniform acceptor density (N_A) and donor density (N_D) doping concentrations for KGeCl3 are being maintained at 10¹⁵cm⁻³ in this simulation. A Current density of 31.02mA/cm² and an output power of 19.04mW/cm² was achieved as indicated in Figure 3 and 4 respectively.

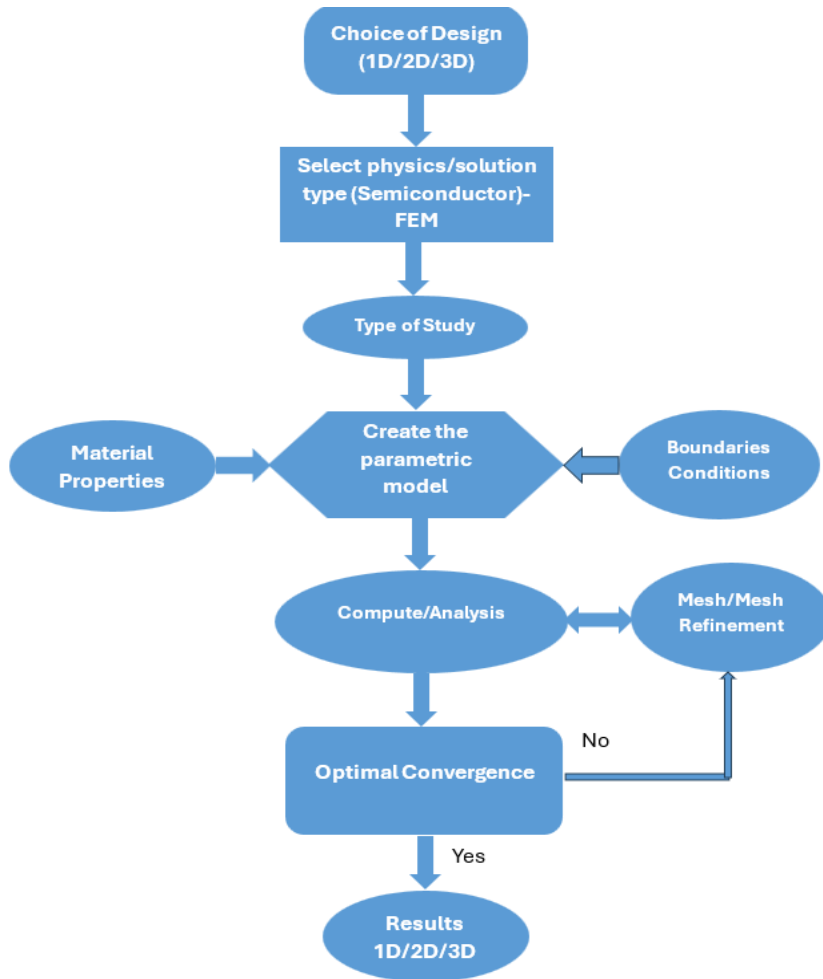


Figure 2. Sequence in COMSOL Multiphysics (Lawal et al, 2025).

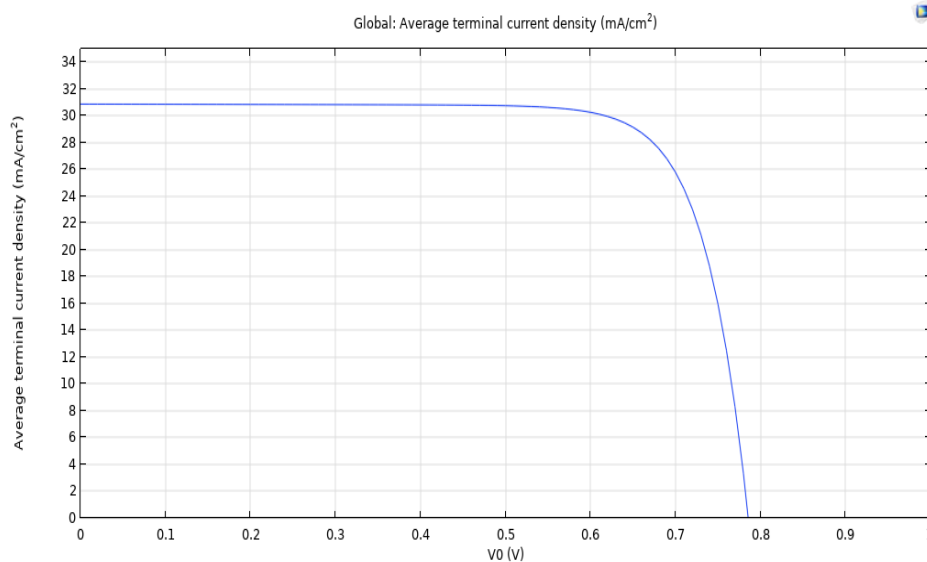


Figure 3. I-V Characteristics of Perovskite Solar Cell

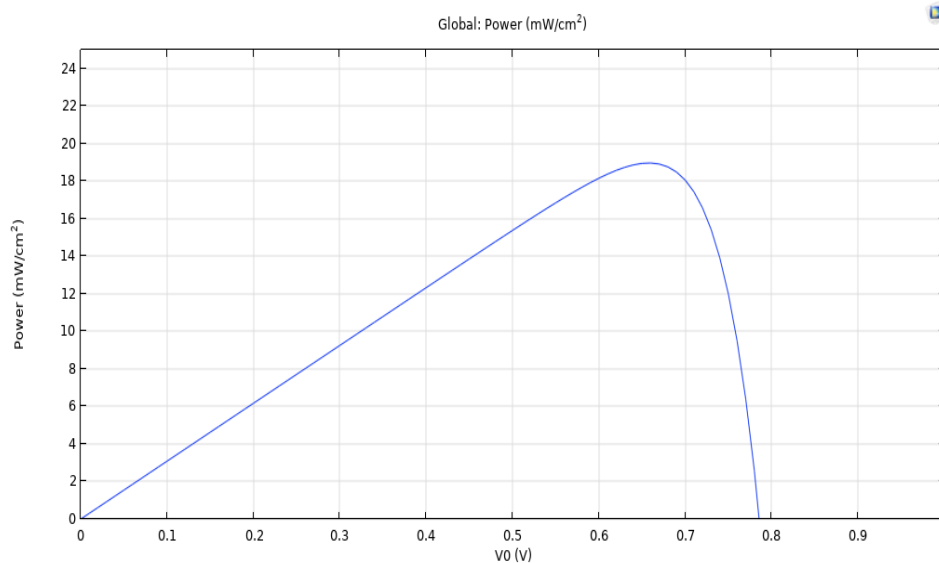


Figure 4. P-V Characteristics of Perovskite Solar Cell

5.0 CONCLUSION

This work has examined the effectiveness and potential of C60 material as an electron transport with a combination of hole transport material in the composition of perovskite solar cells (PSC), while KGeCl₃ in the absorption layer. The absorption material used in this work was potassium germanide chloride (KGeCl₃) and has shown great potential in the power conversion efficiency (PCE) of the PSC solar cell. However, the use of NiO as the hole transport material (HTM) in combination with C60 as electron transport material (ETM) has shown good output results of the PSC solar cells with a current density of 31.02mA/cm² at an open circuit voltage of 0.78V and an output power of 19.04mW/cm²

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Conflicts of Interest

The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, or in the decision to publish the results.

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