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DESIGN AND PERFORMANCE ANALYSIS OF COMPLETE SOLID-STATE DYE SENSITISED SOLAR CELL USING EOSIN-Y XANTHENE DYE: A SCAPS -1D SIMULATION STUDY

K.R. Dhandapani[a,b], N.P. Dhanya[a,c], K. Sebastian Sudheer[a]*
[a]*Department of Physics, Christ College, Irinjalakkuda North, Kerala, India 680125*
[b]*Department of Physics, Govt. Victoria College, Palakkad, Kerala, India 678001*
[c]*Department of Physics, KKTM Govt. College, Pullut, Thrissur, Kerala, India 680663*
**Corresponding Author e-mail: sudheersebastian@christcollegeijk.edu.in*
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This paper reports the theoretical simulation study of the performance of a complete solid-state dye-sensitised solar cell with Eosin-Y as the photosensitizer and PEDOT: PSS as the hole transport layer. SCAPS-1D software is used for the simulation under quasi-ideal conditions and got an optimised efficiency of 4.19%, which matches much with the reported experimental values in the literature. These finding indicates the potential of Eosin-Y as a cost-effective photosensitiser capable of performing even under dim light conditions.
Keywords: *DSSC; Eosin-y; SCAPS-ID; PEDOT:PSS; Simulation*
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1. INTRODUCTION

The growing global energy demand has prompted a shift towards non-conventional sources like solar energy, which offers abundant and constant availability [1]. While silicon solar cells remain prevalent for their efficiency and stability, alternative technologies like dye-sensitized solar cells (DSSCs) show promise despite lower efficiency, suggesting diverse applications in photovoltaics.[2-3]. They operate by sensitizing a wide bandgap semiconductor with a suitable dye, a concept initially proposed by Grätzel and colleagues in 1991, where the use of Ruthenium complexes achieved an efficiency exceeding 10%. Unlike other solar cell types, where semiconducting materials handle multiple functions, DSSCs uniquely utilize dyes for initial light absorption, thus overcoming challenges in obtaining materials with both high light-harvesting and carrier-transporting properties. This dual-material approach in DSSCs allows for independent optimization of spectral properties through dye selection and modification, as well as enhancing carrier transport properties through semiconducting material engineering, offering a more targeted optimization compared to other solar cell technologies [4-5].

The choice of dye significantly impacts DSSC performance, with transition metal coordination compounds offering high efficiencies but posing challenges due to cost and toxicity, leading to research on natural and organic dyes like chlorophylls, flavonoids, and Anthocyanins, which offer advantages of low cost, abundance, and eco-friendliness, with chlorophyll showing notable efficiency of 4.6% in DSSCs [6-9]. Eosin Y, a xanthene dye commonly used due to its high solubility, presents as a red powder with a yellowish tinge and exhibits versatility in various chemical processes [10-13]. While it serves as a cost-effective and environmentally friendly alternative in photocatalysis and functions well in low light, its application in Dye-sensitized solar cells (DSSCs) faces challenges related to stability and efficiency, yet remains promising due to its affordability and versatility compared to Ruthenium complex dyes [14-16].

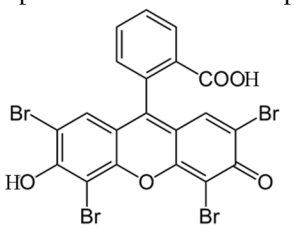

Figure 1. Structure of Eosin

The loading of dye on the photoanode in DSSCs is influenced by the nature and number of anchoring groups, with N3 dye allowing for maximum loading, followed by N719 and Eosin Y. DSSC efficiency, ranging from 0.399% to 5.4%, depends on factors such as dye concentration, photoanode type, electrolyte, and counter electrode; for instance, utilizing Eosin Y with a CuS electrode achieved an efficiency of 7.13%, while our solid-state DSSC attained 4.19% efficiency under quasi-ideal conditions, offering a solution to challenges associated with liquid electrolytes by eliminating concerns like evaporation and leakage, contributing to a reduction in device bulkiness and weight, with hole-transport materials like PEDOT:PSS being utilized in this study [15].

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The design and analysis of the cell are conducted through the use of SCAPS-ID simulation software, an open-source tool developed by Professor M. Burgelman at the University of Gent, Belgium [17]. Employing simulation proves to be a cost-effective and time-efficient approach in contrast to experimental studies. Parameters for layer realization in this study are derived from reported experimental works. Additionally, the software is standardized to yield physically meaningful results by accurately reproducing experimental conditions. The software basically solves five differential equations which are Poisson's equation, continuity equations for electrons and holes, and drift diffusion equations for electrons and holes. In this study, the properties of the hole transport layer (HTL) were optimized, as it is a crucial factor influencing cell performance. Solar cell parameters showed reasonable variation with the thickness and electron affinity of the HTL layer, while other parameters such as acceptor density and trap density remained relatively unchanged compared to the parent cell design based on experimental values from the literature. By utilizing optimized values for the HTL layer, the cell demonstrated improved performance.

Simulation yields V_{oc}, J_{sc}, FF, PCE and also J-V and EQE curves. If the cell is constructed and experiment is carried out to get the above parameters in the real physical situation the results can approach the simulated values based on purity of materials used, fabrication techniques, morphology of layers, optimisation conditions etc.

2. NUMERICAL MODELLING AND DEVICE SIMULATION METHODOLOGY

The solar cell capacitance simulator (SCAPS-ID) is a widely used free software to simulate various types of solar cells.[18], [19] It operates by solving five key differential equations. Through simulation, SCAPS-ID generates comprehensive data, including various solar cell parameters, as well as current-Voltage (JV) and External Quantum Efficiency (EQE) curves.

Operation of solid state DSSC consists of following steps. Dye molecule D get photo excited by absorbing a photon. The molecule D* in the electronically excited state transfer the e^- to the conduction band of photo anode. It is called electron injection and dye become D^+ and it return to electronically ground state. The electrons transferred to C.B. of photo anode move to TCO and are directed to counter electrode through the external load. D^+ acquire e^- from the HTL or give its hole state to hole transport layer (HTL) and get regenerated. HTL take an e- from counter electrode and compensate for its loss. The complete solid state approach make the device more compact by avoiding liquid electrolyte containing redox couple [17, 20,21].

Poisson's equation and electron and hole continuity equations are the starting equations employed by the software [22].

$$\nabla^2\Psi = \frac{q}{\varepsilon}(n - p + N_A - N_D)$$

n= electron concentration, p=hole concentration, ε= absolute permittivity of medium, q=electron charge, ψ= electrostatic potential, N_A= acceptor concentration, N_D= donor concentration

$$\mathbf{\nabla} \cdot \mathbf{J}\mathrm{n} - \mathrm{q}\frac{\partial \mathrm{n}}{\partial \mathrm{t}} = +qR$$

$$\mathbf{\nabla} \cdot \mathbf{J}\mathrm{p} + \mathrm{q}\frac{\partial \mathrm{p}}{\partial \mathrm{t}} = -qR$$

R= carrier recombination rate, $\mathbf{J}_n$= electron current density, **J**p= hole current density

$$\mathbf{J}\mathrm{n} = \mathrm{qn}\mu_n E + qDn\nabla n$$

$$\mathbf{J}\mathrm{p} = \mathrm{qp}\mu_p E - qDp\nabla p$$

E= electric field, Dn= electron diffusion coefficient, Dp= hole diffusion coefficient

Simulation was carried out under AM1.5G spectrum.

3. RESULTS AND DISCUSSIONS

In this study a complete solid state DSSC with Eosin-y as dye sensitizer is designed. TiO_2 is the photo anode and PEDOT: PSS the hole transport material [23]. Gold is used as counter electrode material. The representation of the designed cell and its schematic diagram is given in Figure 2.

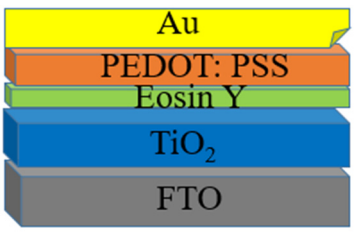

Figure 2. Schematic diagram of the designed cell

The software was validated for this study by reproducing a comparable experimental study. The electrical and optical parameters employed in this simulation are extracted from literature sources in reputable journals. The absorption files and filter files used in the simulation are developed based on data obtained from experimental studies documented in the literature. This approach ensures that the simulation model aligns with established and validated parameters, contributing to the accuracy and reliability of the computational investigation.

Table 1 gives different phot voltaic parameters used for the study.

Table 1. Different parameters used for the study

Parameter	HTL PEDOT:PSS	TiO_2	FTO	Eosin Y
L	500nm	3µm	200nm	5nm
E_g(ev)	2.2	3.2	3.5	2.3[22]
χ(eV)	3.6	3.9	4	3.7
$\in r$	10	9	9	25.3[24]
Nc(cm^{-3})	10^{19}	10^{19}	9.2×10^{18}	2.4×10^{21}
N_V (cm^{-3})	10^{19}	10^{19}	1.8×10^{19}	2.5×10^{21}
Vth(e)	10^7	10^7	10^7	10^7
Vth(h)(cm/s)				
μ_e (cm^2/vs)	100	20	20	10^{-4}
μ_h (cm^2/vs)	0.4	10	24	10^{-4}
N_D(cm^{-3})	0	10^{16}	10^{19}	0
N_A(cm^{-3})	10^{14}	0	0	10^{18}
N_t(cm^{-3})	10^{16}[18]	10^{14} [18]	10^{14} [18]	10^{16} [11], [25]

Work function of back contact 5.1eV ------ [26]
Work function of front contact if 4.8eV-------[22]

Simulation plots are shown in Figure 3.

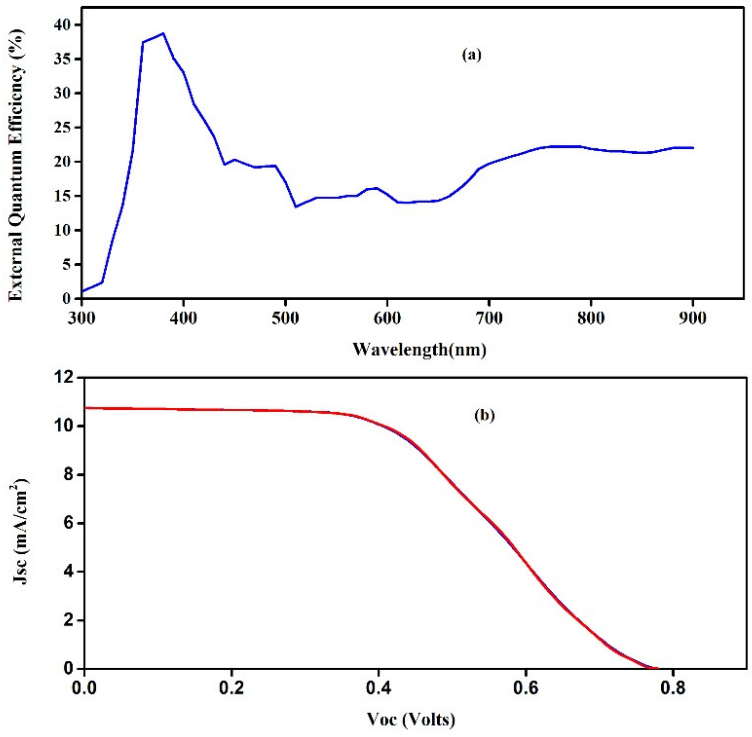

Figure 3. Simulated plots Eosin DSSC (a) EQE with wavelength and (b) J-V curve

To optimize the thickness of the Hole Transport Layer (HTL), a range from 25nm to 500nm was explored via batch calculation simulations. Remarkably, all parameters exhibited their peak values at a thickness of 75nm, thus establishing this dimension as optimal for the HTL in the optimized cell.

Increasing the thickness of the HTL resulted in enhanced light absorption in the longer wavelength region and facilitated a broader pathway for holes originating from the absorber layer to reach the electrode. Consequently, a reduction in hole-electron recombination occurred. These improvements in light absorption and recombination losses were pivotal in elevating solar cell parameters. However, excessively thick HTL layers hindered photon penetration and contributed to increased series resistance within the cell. Moreover, holes faced longer travel distances exceeding their

diffusion length, potentially leading to non-radiative recombination with electrons, thus diminishing solar cell performance when the HTL thickness surpassed the optimum value. The variation of the parameters with HTL thickness is shown in Figure 4.

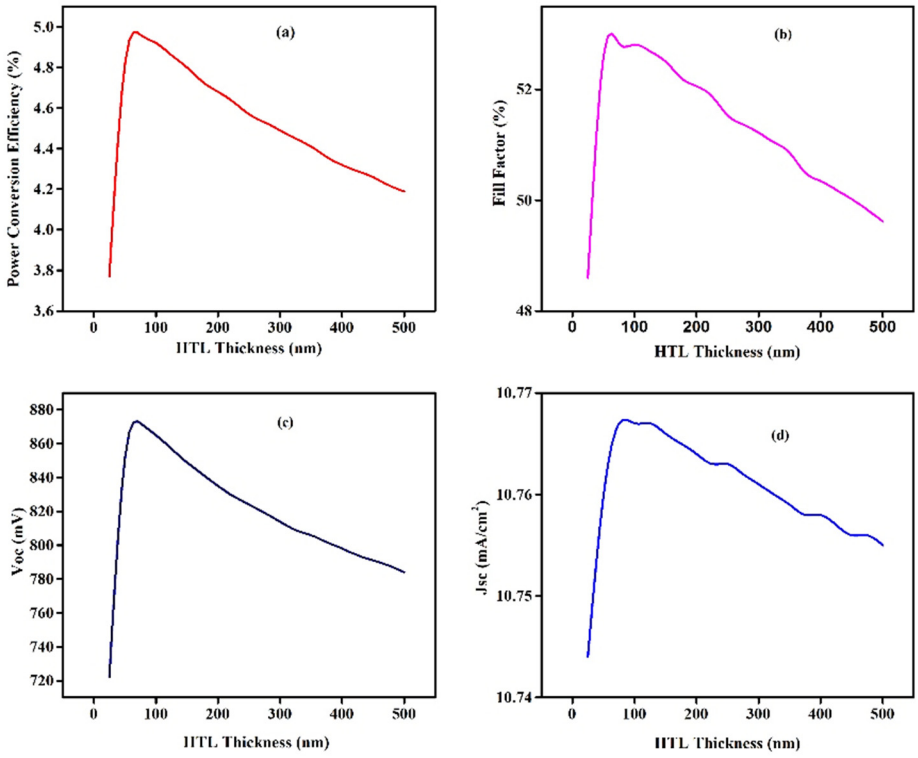

Figure 4. Variation of photovoltaic parameters of the simulated Eosin DSSC (a) PCE with HTL thickness (b) FF with HTL thickness (c) Voc with HTL thickness (d) Jsc with HTL thickness

Exploring electron affinity variations from 3.57eV to 3.63eV revealed optimal cell performance at an affinity of 3.58eV. Unlike thickness variations, the modulation of cell parameters with HTL electron affinity exhibited a gradual and consistent trend.

A higher electron affinity established a greater barrier for electrons at the interface, thereby reducing recombination losses. Additionally, it played a crucial role in aligning energy levels at the HTL/absorber interface, influencing charge carrier dynamics. However, an excessive increase in electron affinity beyond the optimum value hindered hole mobility within the HTL, consequently diminishing overall cell parameters.

a) Variation of Voc with HTL Thickness:

Voc exhibited a remarkable increase from 722 mV to 872 mV as the thickness varied from 25nm to the optimal 75nm. At this optimal thickness, maximum light harvesting and carrier transport were achieved, while recombination losses were minimized.

b) Variation of Jsc with Hole Transport Layer (HTL) thickness:

Jsc showed an increase from 10.744mA/cm² at 25nm to 10.767mA/cm² at the optimal thickness of 75nm, followed by a decline to 10.755mA/cm² at 500nm. Beyond the optimum thickness, reduced Jsc was observed due to significant recombination losses and reduced photon penetration.

c) Variation of Fill Factor (FF) with HTL Thickness:

FF increased from 48.6% at 25nm to a peak of 52.8% at the optimal thickness before declining to 49.6% at 500nm. Elevated recombination rates and increased series resistance at very high HTL thicknesses contributed to the reduction in fill factor.

d) Variation of PCE with HTL Thickness:

Power conversion efficiency surged from 3.77% to 4.96% before decreasing to 4.19% at 500nm. The efficiency peaked at the optimal thickness of 75nm, where maximum light absorption and carrier generation occurred, while excessive thickness led to predominant recombination and resistance losses, causing a decline in efficiency.

e) Variation of Solar Cell Parameters with HTL Electron Affinity:

Voc ranged from 778 mV to 781mV, with a peak at 786mV, while Jsc ranged from 10.754mA/cm² to 10.755 mA/cm², reaching a maximum at 10.756 mA/cm². Similarly, the fill factor varied between 49.2% to 49.7%, with the highest value observed at 49.7%. PCE showed a peak at 4.20%. In all cases, an electron affinity of 3.58 eV was identified as optimal, effectively reducing recombination losses at the HTL/dye interface. The variation of the parameters with electron affinity are shown in Figure 5.

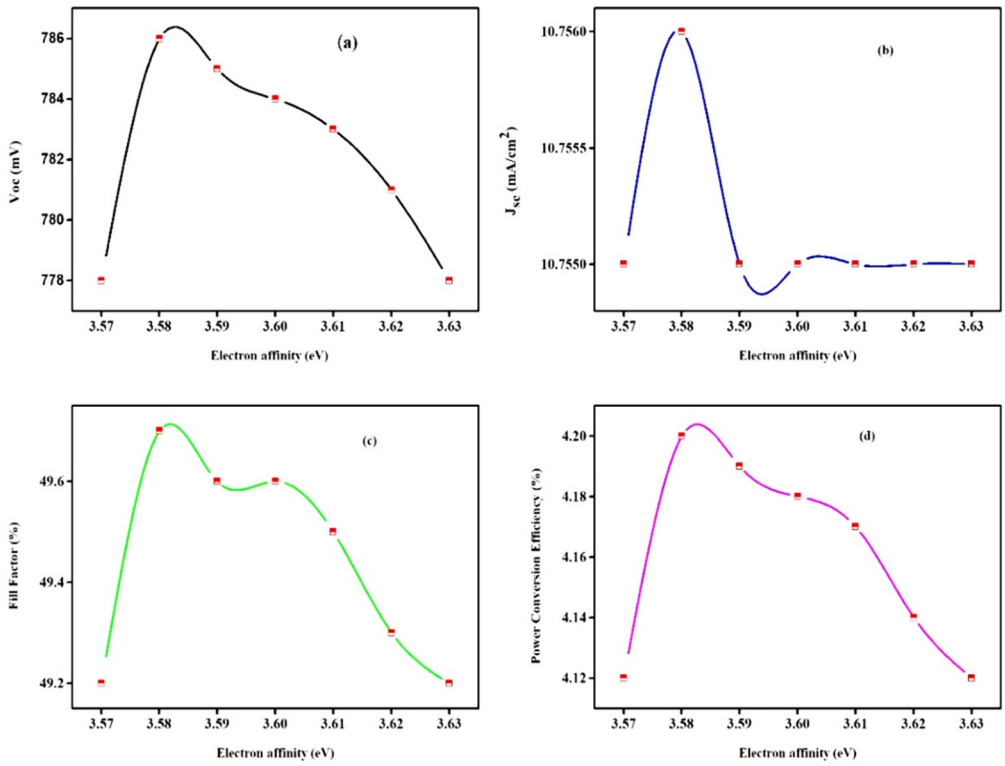

Figure 5. Variation of the photovoltaic parameters with electron affinity
(a) Voc with Electron affinity (b) Jsc with electron affinity (c) FF with electron affinity (d) PCE with electron affinity

Results of the simulated Eosin DSSC are tabulated as given in the Table 2 and optimised parameters are given in Table 3.

Table 2. Simulation results

Parameter	Simulated value
Voc(V)	0.78
Jsc(mA/cm^2)	10.76
FF%	50
PCE%	4.17
Vmax(V)	0.44
Jmax(mA/cm^2)	9.49

Table 3. Optimised parameters

Parameter	After Optimization	Before Optimization
Voc	874 mV	784 mV
Jsc	10.77 mA/cm^2	10.75 mA/cm^2
FF	52.9%	49.6%
PCE	4.97%	4.19%

4. CONCLUSION

This study computationally investigates the effectiveness of Eosin Y dye as a photosensitizer for Dye-sensitized solar cells (DSSC), focusing on a complete solid-state design. Simulated values fall within the range of experimental results, indicating that with careful fabrication and optimization, a practical cell can approach the simulated efficiency. The solid-state design enhances the cell's compactness and portability. Despite lower efficiency and stability compared to Ruthenium complex dyes, Eosin demonstrates potential as a photosensitizer for DSSCs. Further enhancements in efficiency can be achieved through dye modification, selection of a suitable photoanode with appropriate morphology, and optimization of hole transport layer (HTL) and counter electrode materials. Eosin Y's key attributes, including cost-effectiveness, satisfactory light-harvesting capability, ability to perform in low light conditions, and biodegradable and eco-friendly nature, contribute to its appeal in DSSC applications.

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ORCID
K.R. Dhandapani, https://orcid.org/0009-0001-4484-3064, **N.P. Dhanya,** https://orcid.org/0000-0002-4372-2172
K. Sebastian Sudheer, https://orcid.org/0000-0002-9019-4405

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РОЗРОБКА ТА АНАЛІЗ ПРОДУКТИВНОСТІ ПОВНОГО СЕНСИБІЛІЗОВАНОГО НА ТВЕРДОТІЛЬНОГО БАРВНИКА ДЛЯ СОНЯЧНОГО ЕЛЕМЕНТА З ВИКОРИСТАННЯМ ЕОЗИН-Y КСАНТЕНА: ДОСЛІДЖЕННЯ СИМУЛЯЦІЄЮ SCAPS-1D

К.Р. Дхандапані[a,b], Н.П. Дханья[a,c], К. Себастьян Судхір[a]

[a]*Департамент фізики, Християнський коледж, Іріндженалакуда, Керала, Індія 680125*
[b]*Департамент фізики, Урядовий Вікторія коледж, Палаккад, Керала, Індія 678001*
[c]*Департамент фізики, KKTM Урядовий коледж, Пуліт, Трісур, Керала, Індія 680663*

У статті повідомляється про теоретичне моделювання ефективності повного твердотільного сонячного елемента, сенсибілізованого барвником, з Eosin-Y як фотосенсибілізатора та PEDOT: PSS як шару для транспортування дірок. Програмне забезпечення SCAPS-1D використовується для моделювання в квазіідеальних умовах і отримує оптимізовану ефективність 4,19%, що значною мірою відповідає експериментальним значенням, наведеним у літературі. Ці висновки вказують на потенціал Eosin-Y як економічно ефективного фотосенсибілізатора, здатного працювати навіть в умовах слабкого освітлення.

Ключові слова: *DSSC; еозин-у; SCAPS-ID; PEDOT:PSS; симуляція*