

7.379 % POWER CONVERSION EFFICIENCY OF A NUMERICALLY SIMULATED SOLID STATE DYE SENSITIZED SOLAR CELL WITH COPPER (I) THIOCYANATE AS A HOLE CONDUCTOR[†]

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Sourcing for alternative to liquid electrolyte in dye sensitized solar cells (DSSCs) have been the subject of interest in the photovoltaic horizon. Herein, we reported by means of simulation, the performance of dye sensitized solar cell by replacing liquid electrolyte with a copper (I) thiocyanate (CuSCN) hole conductor. The study was carried out using Solar Capacitance Simulation Software (SCAPS) which is based on poisson and continuity equations. The simulation was done based on a n-i-p proposed architecture of FTO/TiO₂/N719/CuSCN/Pt. Result of the initial device gave a Power Conversion Efficiency (PCE), Fill Factor (FF), Short Circuit Current Density (J_{sc}) and Open Circuit Voltage (V_{oc}) of 5.71 %, 78.32 %, 6.23 mAcm⁻², and 1.17 V. After optimizing input parameters to obtain 1×10⁹ cm⁻² for CuSCN/N719 interface defect density, 280 K for temperature, 1.0 μm for N719 dye thickness, 0.4 μm for TiO₂ thickness, Pt for metal back contact, and 0.2 μm for CuSCN thickness, the overall device performance of 7.379 % for PCE, 77.983 % for FF, 7.185 mAcm⁻² for J_{sc} and 1.317 V for V_{oc} were obtained. When compared with the initial device, the optimized results showed an enhanced performance of ~ 1.29 times, 1.15 times, and 1.13 times in PCE, J_{sc} and V_{oc} over the initial device. The results obtained are encouraging and the findings will serve as baseline to researchers involved in the fabrication of novel high-performance solid state DSSCs to realize its appealing nature for industry scalability.

Keywords: ssDSSC, Copper thiocyanate, Hole Conductor, SCAPs

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INTRODUCTION

Issues linked to energy have drawn much research interest due to environmental impact and use of resources that cannot be replenished. Between 80 to 85 % of the global energy used today, comes from fossil fuels which its exploitation results to emission of dangerous pollutants such as nitrous oxide, hydrofluorocarbon, sulfur hexafluoride, carbon dioxide and volatile organic compounds, which has capacity to jeopardize future ecosystem. Photovoltaic has been seen as a promising renewable energy technology that has the ability of converting energy from the sun into electricity with enormous strength to solving problem connected to energy. Since after the report of O'Regan and Grätzel on efficient DSSC [1] based on nanostructured TiO₂ and iodide/tri-iodide (I^-/I^{3-}) redox specie, it has continued to gained attention of global researchers as a potential alternative to widely known silicon solar cell technology. This class of solar cell belongs to the third generation of photovoltaics and has the advantages of simpler production techniques, used of eco-friendly materials and cost effectiveness as compared with its counterpart [2,3].

The DSSC is made up of self-assembled mono-layer of dye in between the wide band gap, otherwise called the electron transport layer and the liquid mediator called the electrolyte [4,5]. However, liquid electrolyte is violent to the surrounding environment it operates which results to corrosive, photo-reactive, and highly volatile nature that affects the sealing status of the DSSCs and consequently, the effect of short-term performance and poor durability of the device is noticed [6]. Sourcing alternative to this liquid electrolyte have been the subject of interest in the photovoltaic horizon [7-9]. The solution to the aforementioned challenges is to replace the liquid electrolyte with solid state p-type semiconductor, this will take care of the leakage, heavy weight and architectural complexity.

The structure of a solid-state dye sensitized solar cell is depicted in Figure 1 [10], which shows its working principle. The dye absorbs photon energy, and then promote electron to the conduction band of the dye, and subsequently the electrons are transferred to the conduction band of the TiO₂. The dye that has lost electron regenerates through the process of hole injection from hole transport material. The electrons promoted to the TiO₂ conduction band flow through the network and are collected at the FTO and the holes within the hole transport material are collected at the counter electrode.

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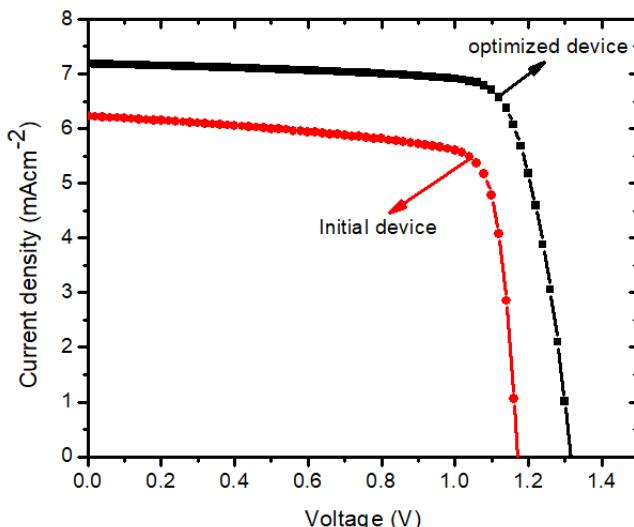


Figure 14. Combine J-V curves for the initial and optimized device

CONCLUSION

We reported the performance of a solid state dye sensitized solar cell based on CuSCN as a hole conductor using SCAPS-1D. The performance of the overall ssDSSC was achieved by optimizing the CuSCN/dye interface defect, operating temperature, CuSCN thickness, TiO₂ thickness and N719 dye thickness through data variation. The optimized device results to 7.379 % PCE, 77.983 % FF, 7.185 mAcm⁻² Jsc and 1.317 V Voc. This research suggests that, efficient stable and durable dye sensitized solar cells can be achieved by replacing liquid electrolyte with CuSCN hole conductor that is cost effective.

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REFERENCES

- [1] B. O'regan, and M. Grätzel, *Nature*, **353**, 737–740 (1991), <https://doi.org/10.1038/353737a0>
- [2] S. Sharma, K.K. Jain, and A. Sharma, *Materials Sciences and Applications*, **6**(12), 1145–1155 (2015), <https://doi.org/10.4236/msa.2015.612113>
- [3] V.R. Gómez, F.A. Mató, D.S. Jiménez, G.S. Rodríguez, A.Z. Lara, I.M. De Los Santos, and H.Y.S. Hernández, *Optical and Quantum Electronics*, **52**, 324 (2020), <https://doi.org/10.1007/s11082-020-02437-y>
- [4] A. Hagfeldt, G. Boschloo, L.C. Sun, L. Kloo, and H. Pettersson, *Chemical Reviews*, **110**, 6595–6663 (2010), <https://doi.org/10.1021/cr000356p>
- [5] M. Gratzel, *Accounts of Chemical Research*, **42**, 1788–1798 (2009), <https://doi.org/10.1021/ar900141y>
- [6] S. Yanagida, Y.H. Yu, and K. Manseki, *Accounts of Chemical Research*, **42**, 1827–1838 (2009), <https://doi.org/10.1021/ar900069p>
- [7] I. Chung, B. Lee, J. He, R.P.H. Chang, and M.G. Kanatzidis, *Nature*, **485**, 486–489 (2012), <https://doi.org/10.1038/nature11067>
- [8] M. Wang, N. Chamberland, L. Breau, J.E Moser, R.H. Baker, B. Marsan, S.M. Zakeeruddin, and M. Grätzel, *Nature Chemistry*, **2**, 385–389 (2010), <https://doi.org/10.1038/nchem.610>
- [9] A. Yella, H.W. Lee, H.N. Tsao, C. Yi, A.K. Chandiran, M.K. Nazeeruddin, E.W.G. Diau, C.Y. Yeh, S.M. Zakeeruddin, and M. Grätzel, *Science*, **334**, 629–634 (2011), <https://doi.org/10.1126/science.1209688>
- [10] K.H. Wong, K. Ananthanarayanan, S.R. Gajjela, and P. Balaya, *Materials Chemistry and Physics*, **125**, 553–557 (2011), <https://doi.org/10.1016/j.matchemphys.2010.10.017>
- [11] F. Jahantigh, and M.J. Safkhani, *Applied Physics A*, **125**, 276 (2019), <https://doi.org/10.1007/s00339-019-2582-0>
- [12] L. Schmidt-Mende, S.M. Zakeeruddin, and M. Grätzel, *Applied Physics Letters*, **86**, 013504 (2005), <https://doi.org/10.1063/1.1844032>
- [13] W. Zhang, Y. Cheng, X. Yin, and B. Liu, *Macromolecular Chemistry and Physics*, **212**, 15–23 (2011), <https://doi.org/10.1002/macp.201000489>
- [14] F. Arith, O.V. Aliyaselvam, A.N.M. Mustafa, M.K. Nor, and O.A. Al-Ani, *International journal of renewable energy research*, **11**(2), 869–878 (2021), <https://www.ijrer.org/ijrer/index.php/ijrer/article/view/12046/pdf>
- [15] E.V.A. Premalal, G.R.R.A. Kumara, R.M.G. Rajapakse, M. Shimomura, K. Murakami, and A. Konno, *Chemical Communication*, **46**, 3360–3362 (2010), <https://doi.org/10.1039/B927336K>

- [16] R. Hehl, and G. Thiele, Anorganische und Allgemeine Chemie, **626**, 2167–2172 (2000), [https://doi.org/10.1002/1521-3749\(200010\)626:10%3C2167::AID-ZAAC2167%3E3.0.CO;2-7](https://doi.org/10.1002/1521-3749(200010)626:10%3C2167::AID-ZAAC2167%3E3.0.CO;2-7)
- [17] V. Perera, and K. Tennakone, Solar Energy Materials and Solar Cells, **79**(2), 249–255 (2003), [https://doi.org/10.1016/S0927-0248\(03\)00103-X](https://doi.org/10.1016/S0927-0248(03)00103-X)
- [18] B.K. Korir, J.K. Kibet, and S.M. Ngari, Optical and Quantum Electronics, **53**, 368 (2021), <https://doi.org/10.1007/s11082-021-03013-8>
- [19] M. Burgelman, J. Verschraegen, S. Degrave, and P. Nollet, Progress in Photovoltaics: Research and Applications, **12**(2–3), 143–153 (2004), <https://doi.org/10.1002/pip.524>
- [20] D. Bartesaghi, I. del Carmen Pérez, J. Kniepert, S. Roland, M. Turbiez, D. Neher, and L.J.A. Koster, Nature Communications, **6**(1), 1–10 (2015), <https://doi.org/10.1038/ncomms8083>
- [21] E.V.A. Premalal, N. Dematage, and A. Konno, Chemistry Letters, **41**, 510–512 (2012), <https://doi.org/10.1246/cl.2012.510>
- [22] A.M. Karmalawi, D.A. Rayan, and M.M. Rashad, Optik, **217**, 164931 (2020), <https://doi.org/10.1016/j.ijleo.2020.164931>
- [23] A.J. McEvoy, L. Castaner, T. Markvart, in: *Solar cells: materials, manufacture and operation*, (Academic Press, Amsterdam, 2013), pp. 3–25.
- [24] N. Devi, K.A. Parrey, A. Aziz, and S. Datta, Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures Processing, Measurement, and Phenomena, **36**(4), 04G105 (2018), <https://doi.org/10.1116/1.5026163>
- [25] Y. Gan, X. Bi, Y. Liu, B. Qin, Q. Li, Q. Jiang, and P. Mo, Energies, **13**(22), 5907 (2020), <https://doi.org/10.3390/en13225907>
- [26] A.K. Daoudia, Y. El Hassouani, and A. Benami, International Journal of Engineering and Technical Research, **6**(2), 71–75 (2016), <https://www.academia.edu/download/54231833/IJETR042544.pdf>
- [27] U. Mehmood, A. Al-Ahmed, F.A. Al-Sulaiman, M.I. Malik, F. Shehzad, and A.U.H. Khan, Renewable and Sustainable Energy Reviews, **79**, 946 (2017), <https://doi.org/10.1016/j.rser.2017.05.114>
- [28] P. Roy, S. Tiwari, and A. Khare, Results in Optics, **4**, 100083 (2021), <https://doi.org/10.1016/j.rio.2021.100083>
- [29] S. Dubey, J.N. Sarvaija, and B. Seshadri, Energy Procedia, **33**, 311–321 (2013), <https://doi.org/10.1016/j.egypro.2013.05.072>
- [30] A. Shahriar, S. Hasnath, and M.A. Islam, EDU Journal of Computer and Electrical Engineering, **01**(01), 31–37 (2020), <https://doi.org/10.46603/ejcee.v1i1.21>
- [31] C. Xiang, X. Zhao, L. Tan, J. Ye, S. Wu, S. Zhang, and L. Sun, Nano Energy, **55**, 269–276 (2019), <https://doi.org/10.1016/j.nanoen.2018.10.077>
- [32] W. Cai, Z. Zhang, Y. Jin, Y. Lv, L. Wang, K. Chen, and X. Zhou, Solar Energy, **188**, 441–449 (2019), <https://doi.org/10.1016/j.solener.2019.05.081>
- [33] N.A. Bakr, A.K. Ali, S.M. Jassim, and K.I. Hasoon, ZANCO Journal of Pure and Applied Sciences, **29**(s4), s274–s280 (2017), <https://doi.org/10.21271/ZJPAS.29.s4.31>
- [34] J.M.K.W. Kumari, N. Sanjeevadharshini, M.A.K.L. Dissanayake, G.K.R. Senadeera, and C.A. Thotawatthage, Ceylon Journal of Science, **45**(1), 33–41 (2016), <http://dx.doi.org/10.4038/cjs.v45i1.7362>
- [35] D.L. Domtau, J. Simiyu, E.O. Ayieta, L.O. Nyakiti, B. Muthoka, and J.M. Mwabora, Surface Review and Letters, **24**(5), 1750065 (2017), <https://doi.org/10.1142/S0218625X17500652>
- [36] Z.S. Wang, H. Kawauchi, T. Kashima, and H. Arakawa, Coordination Chemistry Reviews, **248**, 1381–1389 (2004), <https://doi.org/10.1016/j.ccr.2004.03.006>
- [37] M.C. Kao, H.Z. Chen, S.L. Young, C.Y. Kung, and C.C. Lin, Thin Solid Films, **517**, 5096–5099 (2009), <https://doi.org/10.1016/j.tsf.2009.03.102>
- [38] F. Behrouznejad, S. Shahbazi, N. Taghavinia, H.P. Wu, and E. W-G. Diau, Journal of Materials Chemistry A, **4**, 13488–13498 (2016), <https://doi.org/10.1039/C6TA05938D>

7,379 % ЕФЕКТИВНІСТЬ ПЕРЕТВОРЕННЯ ЕНЕРГІЇ ЧИСЛЕННО ЗМОДЕЛЬОВАНОГО ТВЕРДОГО СОНЯЧНОГО ЕЛЕМЕНТУ СЕНСИБІЛІЗОВАНОГО БАРВНИКОМ З ТІОЦІНАТОМ МІДІ (І) У ЯКОСТІ ДІРКОВОГО ПРОВІДНИКА

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Предметом дослідження був пошук альтернативи рідкому електроліту в сонячних елементах, сенсибілізованих барвником (DSSC), щодо фотоелектрических властивостей. Тут шляхом моделювання ми повідомили про продуктивність сонячного елемента, сенсибілізованого барвником, замінивши рідкий електроліт на дірковий провідник з мідного (І) тіоцианату^z(CuSCN). Дослідження проводилося за допомогою програмного забезпечення для моделювання сонячної емності (SCAPS), яке базується на рівняннях Пуассона та безперервності. Моделювання проводилося на основі запропонованої n-i-p архітектури FTO/TiO₂/N719/CuSCN/Pt. Результат початкового пристрою дав ефективність перетворення потужності (PCE) - 78,32 %, коефіцієнт заповнення (FF) - 5,71 %, щільність струму короткого замикання (J_{sc}) - 6,23 mAcm⁻², і напругу холостого ходу (Voc) - 1,17 V. Після оптимізації вхідних параметрів для отримання 1×109 см⁻² для щільноти дефектів інтерфейсу CuSCN/N719, 280 K для температури, 1,0 мкм для товщини барвника N719, 0,4 мкм для товщини TiO₂, Pt для зворотного контакту металу та 0,2 мкм для товщини CuSCN, було отримано загальну продуктивність пристрою 7,379 % для PCE, 77,983 % для FF, 7,185 mAcm⁻² для J_{sc} та 1,317 V для Voc. У порівнянні з початковим пристроєм, оптимізовані результати показали покращену продуктивність приблизно в 1,29 рази, 1,15 рази та 1,13 рази в PCE, J_{sc} і Voc порівняно з початковим пристроєм. Отримані результати є обнадійливими, і одержані дані можуть послужити базою для дослідників, які беруть участь у виготовленні нових високопродуктивних твердотільних DSSC, щоб зрозуміти їхню привабливість для масштабованості в галузі.

Ключові слова: ssDSSC, тіоцианат міді, дірковий провідник, SCAPs