Performance Evaluation of Zinc-Phthalocyanine as an Active Material in Dye-Sensitized Solar Cells

Ghazi Aman Nowsherwan[1], Mohsin Khan[1], Muhammad Ahmad[1], Syed Sajjad Hussain[1], Saira Riaz[1], Shahzad Naseem[1]

[1]Centre of Excellence in Solid State Physics, University of the Punjab, Lahore 54590, Pakistan

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ABSTRACT

The increase of global energy consumption and the related ecological problems have generated a constant demand for alternative energy sources superior to traditional ones. This is why unlimited photon-energy harnessing is important. A notable focus to address this concern is on advancing and producing cost-effective low-loss solar cells. For efficient light energy capture and conversion, we fabricated a ZnPC: PC70BM-based dye-sensitized solar cell (DSSC) and estimated its performance using a solar cell capacitance simulator (SCAPS-1D). We evaluated the output parameters of the ZnPC: PC70BM-based DSSC with different photoactive layer thicknesses, series and shunt resistances, and back-metal work function. Our analyses show that moderate thickness, minimum series resistance, high shunt resistance, and high metal-work function are favorable for better device performance due to low recombination losses, electrical losses, and better transport of charge carriers. In addition, indepth research for clarifying the impact of factors, such as thickness variation, defect density, and doping density of charge transport layers, has been conducted. The best efficiency value found was 10.30% after tweaking the parameters. It also provides a realistic strategy for efficiently utilizing DSSC cells by altering features that are highly dependent on DSSC performance and output.

DESIGN AND METHOD

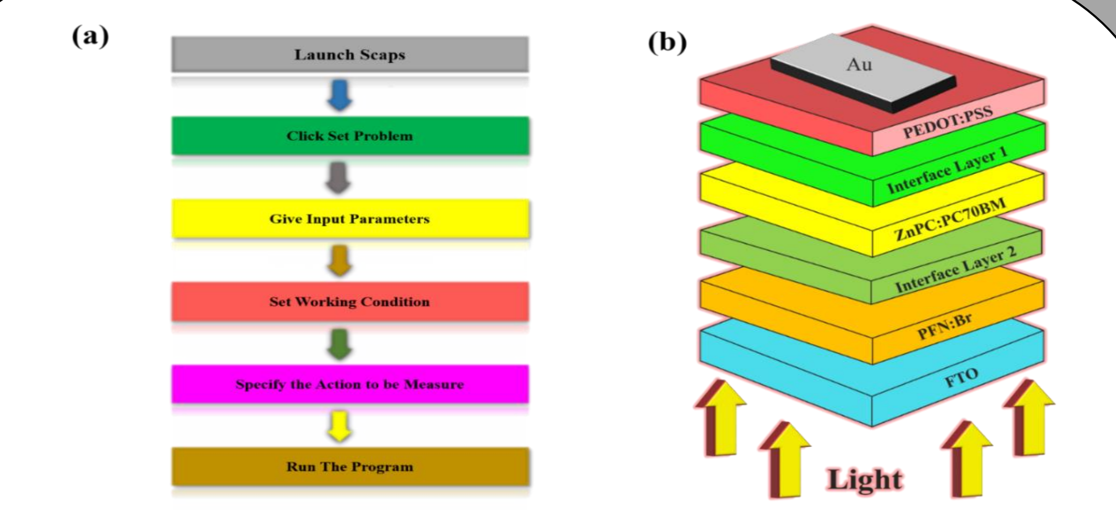

Figure 1. (a) Basic steps for numericalization SCAPS-1D, and (b) A diagrammatic representation of the intended DSSC structure

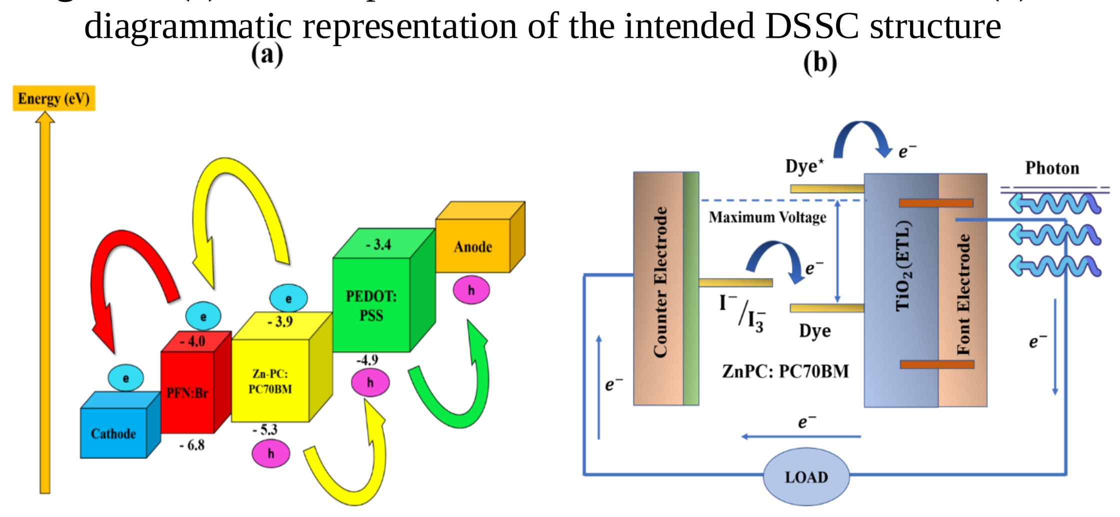

Figure 2. (a) HOMO-LUMO band diagram of the proposed DSSC, and (b) Schematic of operation principle of DSSC.

PHOTOACTIVE CURRENT DENSITY AND QUANTUM EFFICIENCY RESPONSE

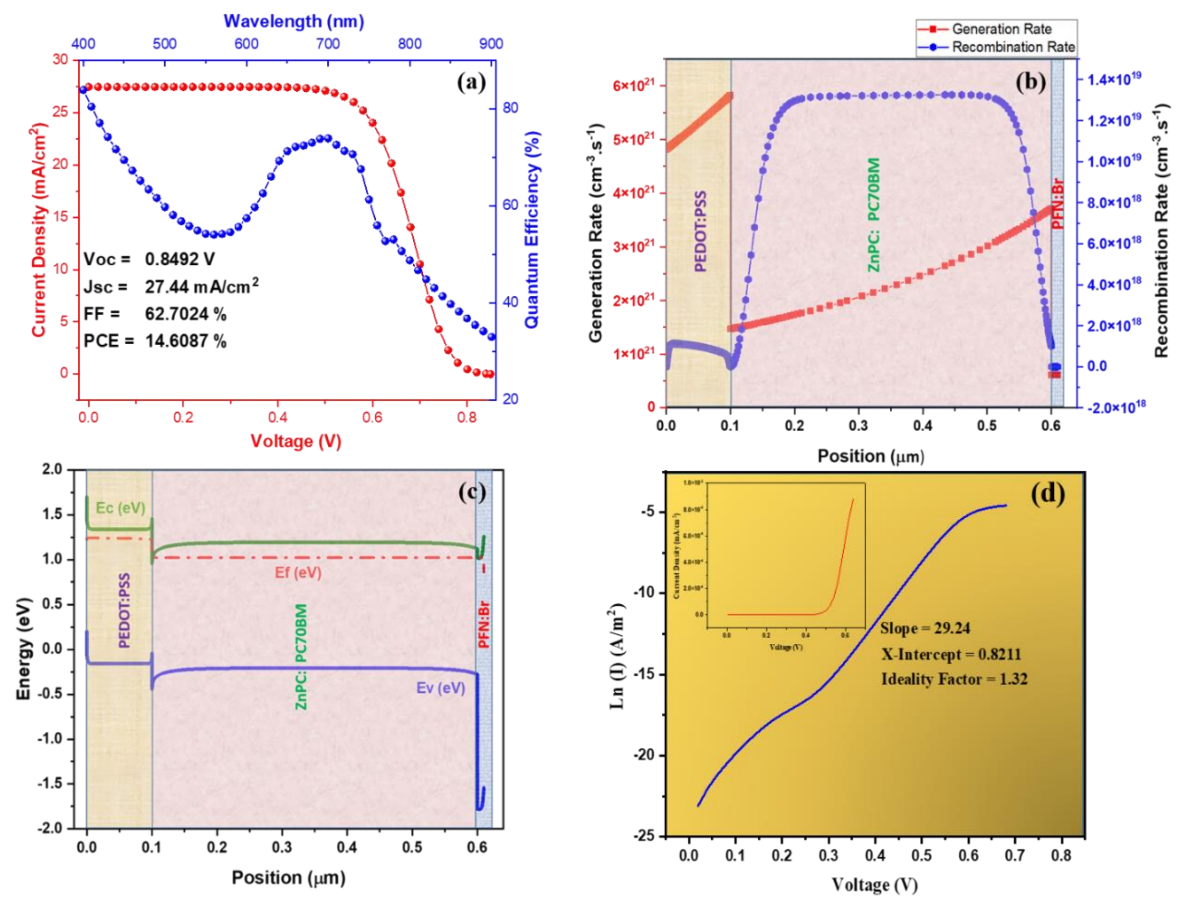

Figure 3. (a) J-V and QE curve of the intended device (b) Generation and recombination rate of photogenerated carriers in device (c) Energy band structure of purposed device, and (d) Ln (I) vs Voltage (Inset represents Dark J-V Measurement).

INFLUENCE OF ACTIVE LAYER THICKNESS ON CELL FUNCTIONALITY

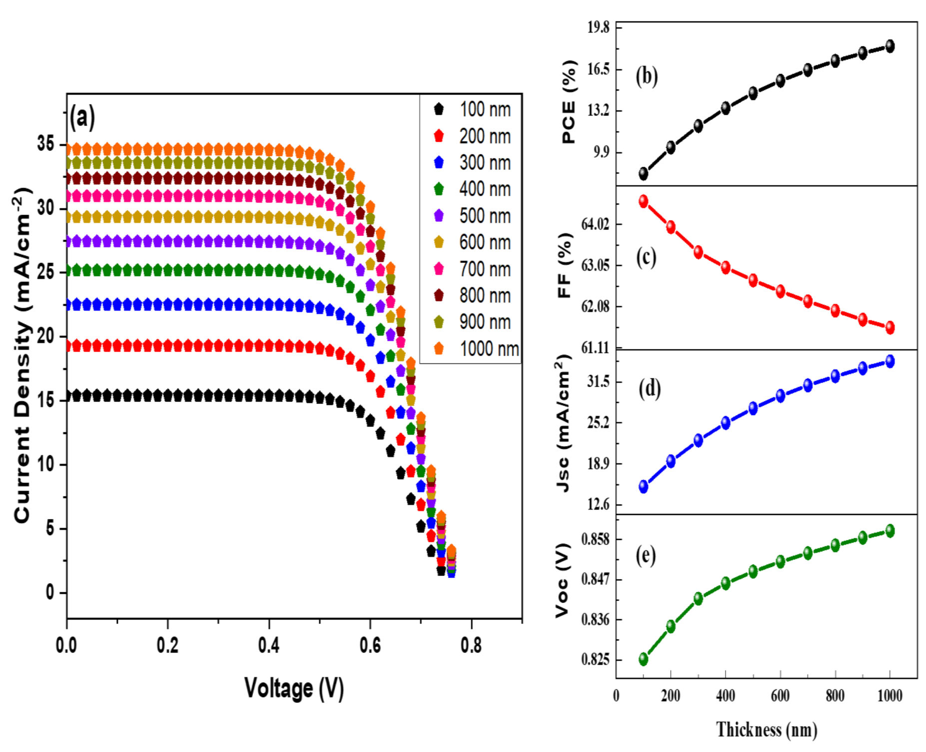

Figure 4. (a) J-V comparison at different values of thickness, (b) PCE, (c) FF, (d) Jsc, and (e) Voc in relation to photoactive layer thickness.

INFLUENCE OF SERIES AND SHUNT RESISTANCE ON CELL FUNCTIONALITY

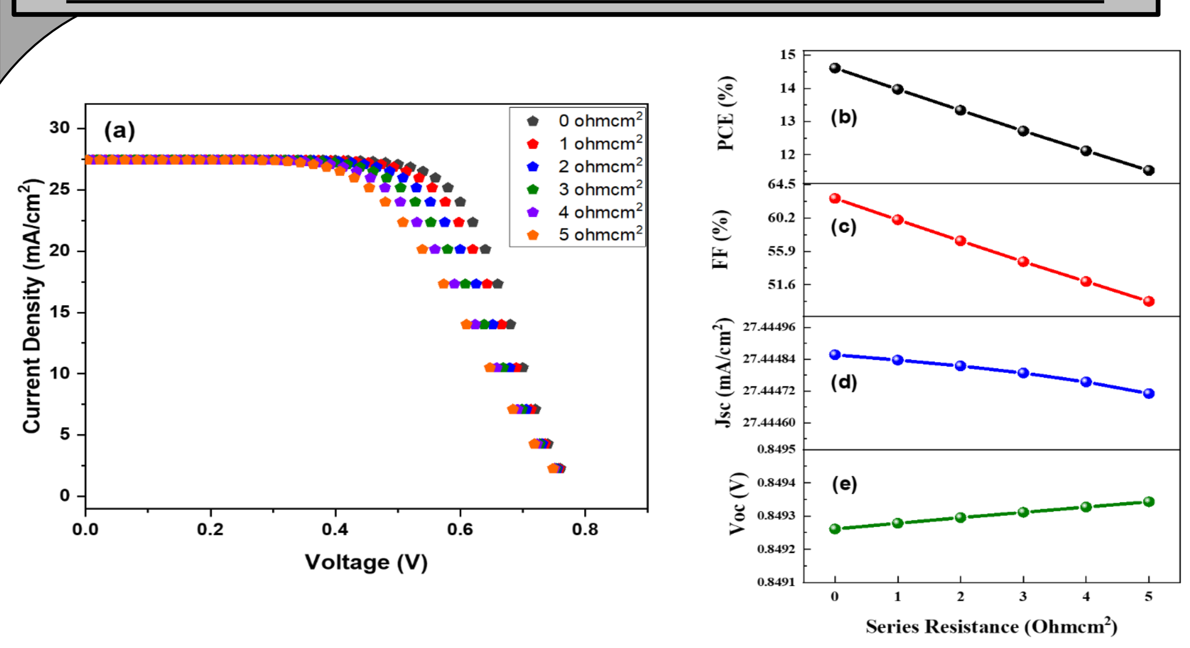

Figure 5. (a) J-V comparison at different values of series resistance, (b) PCE, (c) FF, (d) Jsc, and (e) Voc in relation to series resistance.

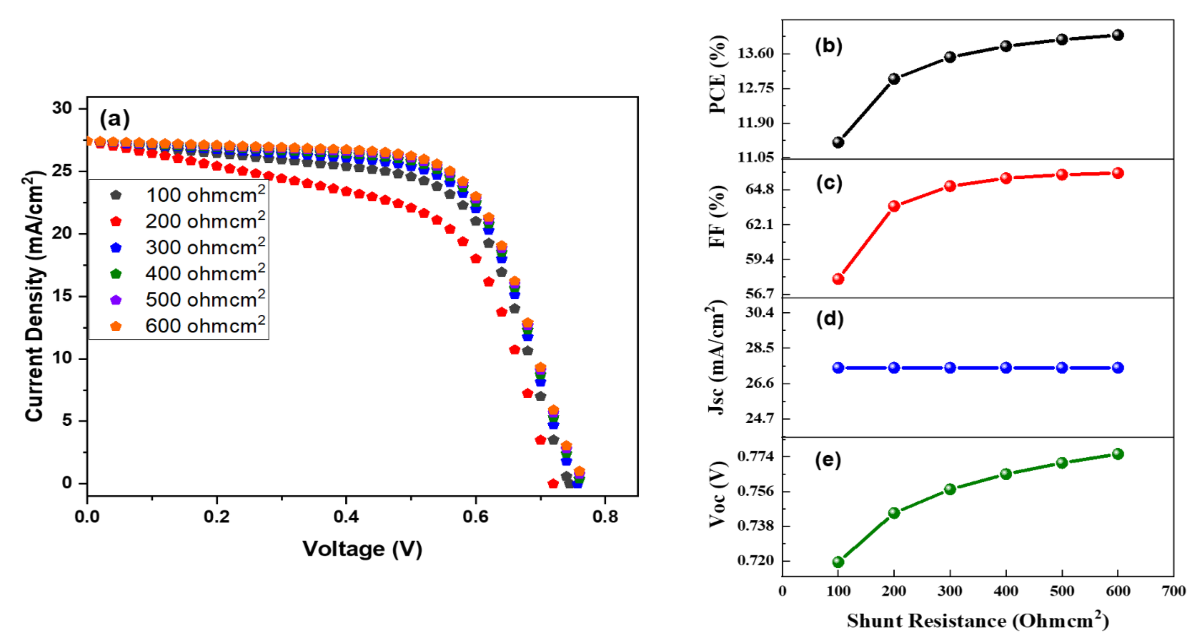

Figure 6. (a) J-V comparison at different values of Shunt resistance, (b) PCE, (c) FF, (d) Jsc, and (e) Voc in relation Shunt resistance.

INFLUENCE OF DEFECT DENSITY OF PHOTOACTIVE LAYER ON CELL FUNCTIONALITY

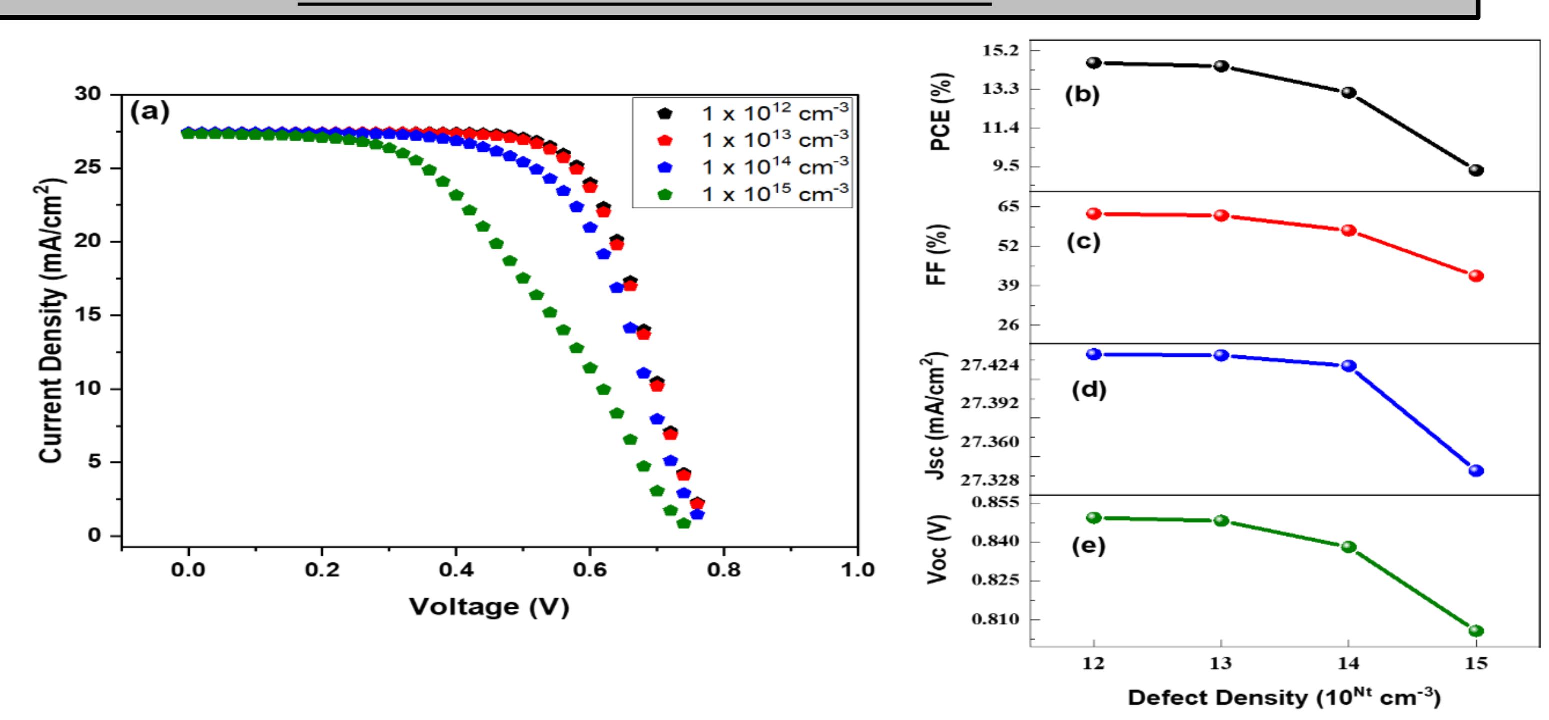

Figure 7. (a) J-V comparison at different values of defect mobility, (b) PCE, (c) FF, (d) Jsc, and (e) Voc

INFLUENCE OF VARYING BACK METAL CONTACT ON DEVICE PERFORMANCE

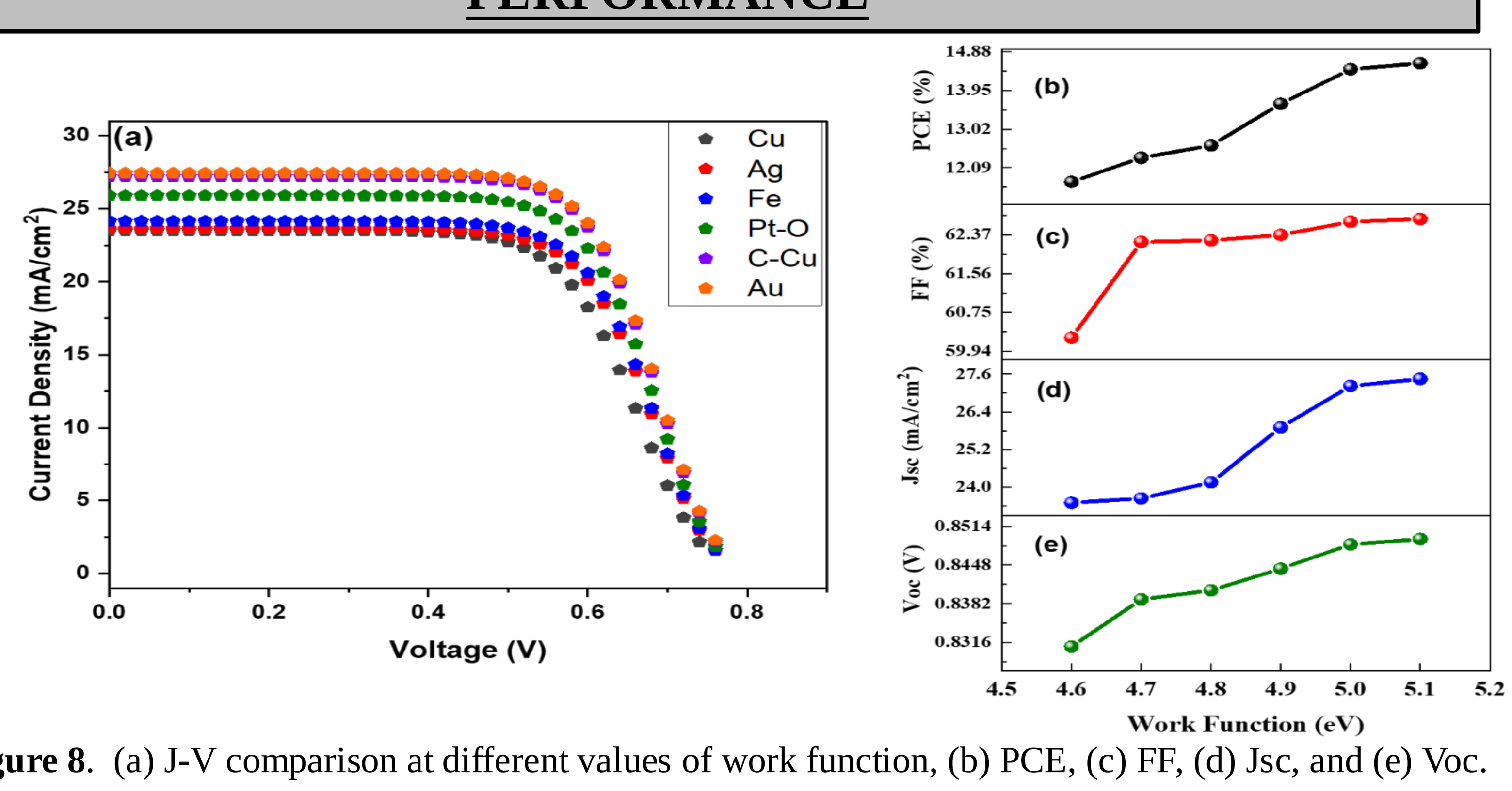

Figure 8. (a) J-V comparison at different values of work function, (b) PCE, (c) FF, (d) Jsc, and (e) Voc.

COMPARISON OF SIMULATED RESULT WITH EXPERIMENTAL RESULTS

Device Configuration	PCE (%)	Ref.
Experimental Results		
4-HBa-ZnPc	2.99	[65]
4-MKBa-CoPc	4.18	[66]
FTO/TiO_2/N719/CuSCN/C	4.24	[66]
P3HT:PCBM/ZnPC	5.3	[67]
FTO/TiO_2/ $CsPbBr_3$:ZnPc/C	7.67	[68]
FTO/TiO_2/ $CsPbBr_3$/ZnPc:P3HT/C	10.03	[68]
FTO/dye & TiO_2 (TNA)/Pt	8.34	[69]
ITO/PEDOT:PSS/PTB7:ZnPc:PC71BM/Ca	8.52	[70]
PTB7:PC70BM	9.55	[71]
Simulation Results		
FTO/PFN:Br/ZnPC:PC70BM (200nm)/PEDOT:PSS/Au	10.29	This study
FTO/PFN:Br/ZnPC:PC70BM (500nm)/PEDOT:PSS/Au	14.61	This study

CONCLUSION

- This work has offered valuable insights into how the characteristics of DSSCs might be altered during the commercial manufacture of solar cells.
- The SCAPS-1D software package is utilised to optimize and design the desired DSSC structure: FTO/PFN:Br/Active Material/PEDOT:PSS/Au.
- The cell performance was maximized by making suitable modifications to thickness, series and shunt resistances, metal-contact work functions, carrier mobility, and different trap density.
- The analysis shows that the material's photovoltaic properties have improved by reducing the defect density, by adjusting the absorber layer thickness appropriately, and by raising the charge carrier mobility.
- According to our findings, the best value for thickness is 500 nm, for defect density is 1 × 10^{12} cm^{-3}, and for carrier mobility is 5 cm^2/Vs to achieve high productivity. By optimizing all the prime parameters, we could construct DSSC with high efficiency of 14.61 % and the simulated result suggests that the performance of DSSC devices will increase in the near future.