

## ABSTRACT

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Climate change has approached a major crisis limit worldwide due to exhaust emissions arising from the use of traditional transport fuels. Solar energy, therefore, appears to be the most promising alternative energy that can mitigate air quality and environmental degradation. Herein, we report numerical simulation of a novel model solid-state dye-sensitized solar cell consisting of solid-state layers with the configuration FTO/PC<sub>61</sub>BM/N719/CuSCN/Au using 1-dimensional solar cell capacitance simulator software (SCAPS-1D). The motivation underpinning the numerical simulation of the solar cell architecture proposed in this study was to optimize phenyl-C61-butyric acid methyl ester (PC<sub>61</sub>BM) performance as the electron transport layer. In this model, the effects of varying several parameters—temperature, absorber thickness, defect density, and metallic back contact on the overall solar cell performance have been critically examined. After optimizing the input parameters, the optimal conversion efficiency was 5.38% while the optimized open-circuit voltage was 0.885 V. Besides, 70.94% was the optimum fill factor and the peak short-circuit current of 8.563 mA cm<sup>-2</sup> was achieved. Built-in voltage of ~ 1.0 V was estimated from the Mott–Schottky curve and the cell band diagram. The power conversion efficiency obtained in this study is robust for this cell configuration, and is toxic-free compared to the lead-based perovskite solar cells. These findings are therefore useful in the advancement and fabrication of high-performance dye-based photovoltaic devices for large-scale industrial production.