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Effect of Ce_2O_3-Based ETL for High-Efficiency Lead-Free Perovskites

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The search for lead-free, highly efficient solar systems has attracted attention towards novel materials and interface design. Using Ce_2O_3 as the electron transport layer and Cs_2PtI_6 as the lead-free absorber, this work numerically analyses a perovskite-inspired solar cell organised as ITO/Ce_2O_3. Using SCAPS-1D simulations, two fundamental parameters Cs_2PtI_6 absorber thickness and the relative dielectric permittivity (ϵ_r) of important layers were systematically evaluated. With its broad band gap, favourable conduction band alignment, and chemical stability, the Ce_2O_3 layer greatly enhanced charge extraction and reduced recombination. Optimal thickness of 1.5–1.6 μm was found to be Cs_2PtI_6, which balanced carrier transport with light absorption. Furthermore, by encouraging exciton dissociation and thereby enhancing dielectric screening, increasing the ϵ_r of the Cs_2PtI_6 layer produced significant increases in V_{oc}, J_{sc}, FF, and PCE. The best device obtained an open-circuit voltage (V_{oc}) of 1.20265 V, a short-circuit current density (J_{sc}) of 32.22 mA/cm², a power conversion efficiency (PCE) of 31.07%, and a fill factor (FF) of 80.17%. These findings underline the need of thickness control, dielectric optimisation, and material selection, especially the integration of Ce_2O_3, in the evolution of effective, stable, and environmentally friendly solar systems.

Keywords: Perovskite solar cell, Ce_2O_3, Cs_2PtI_6, CNTs, lead-free photovoltaics, SCAPS-1D simulation, power conversion efficiency

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The growing urgency of climate change, coupled with the world's rising energy demands, has intensified the search for clean and renewable energy solutions. The worldwide movement towards sustainable energy systems has acquired important momentum as carbon dioxide emissions rise and fossil fuel sources run out. Among the renewable sources, solar energy is one of the most exciting ones as it is plentiful, readily accessible, and generally acknowledged to be able to satisfy future demands. Thanks to its dependability, scalability, and low environmental impact, solar photovoltaic (PV) technology has become quite important in this change [1]. According to projections [2], suggest that for the next two decades solar power might account for up to 20% of the main energy source worldwide. PV's potential to be used across a variety of geographical areas, its renewable character, and its vital part in lowering greenhouse gas emissions drive this expected increase. PV technology is crucial in the worldwide endeavour to reach carbon neutrality and fight climate change as it offers a clean and sustainable road ahead, unlike those of traditional fossil fuel-based systems [3].

Over the last thirty years, a lot of study has been done to improve the design and efficiency of semiconductor-based solar cells. Silicon is still the main component used in commercial solar technologies in significant part because to its well-established production methods and quite high conversion efficiency. Rising production costs, mostly related to the energy-intensive purification and processing phases, along with the strict quality criteria needed for maximum performance, restrict the overall usage of silicon-based solar cells.[4]. Even though silicon device efficiency has improved, cost-related challenges still exist and prevent their broad implementation [5]. This has spurred further research on alternative materials that strike a compromise between cost-effective performance. The great capacity of perovskite-structured materials in offering effective and cheap solar energy conversion has attracted attention. The development of next-generation

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photovoltaic technology depends on a practical and scalable basis that perovskite solar cells are providing [6].

Kojima et al. initially showed the utilization of perovskite materials in photovoltaics, achieving an initial PCE of 3.8% [7]. In the last 10 years, rigorous research and materials engineering have enhanced this efficiency to about 25.5%, positioning perovskites as a leading contender in solar energy. The inclusion of lead (Pb) in most high-efficiency perovskite formulations raises substantial environmental and health issues, creating formidable obstacles to their large-scale commercial implementation [8, 9]. Researchers have investigated alternate divalent metal cations, including tin (Sn^{2+}) and germanium (Ge^{2+}), which possess similar oxidation states and electronic configurations to lead. These constituents provide possible avenues for the creation of lead-free, ecologically friendly perovskite absorbers [10-12].

Calcium platinum iodide (Cs_2PtI_6), a lead-free halide double perovskite, has surfaced as a viable choice for ecologically sustainable and stable light-absorbing materials in photovoltaic applications. Cs_2PtI_6 has a straight bandgap of around 1.37 eV, making it ideal for single-junction solar cells and facilitating effective absorption over a broad range of the solar spectrum. Apart from its optimal bandgap, Cs_2PtI_6 shows a noteworthy absorption coefficient and prolonged minority carrier lifetime—both crucial elements for achieving high PCE [13]. Promising results from experimental validations have come from prototype devices utilising Cs_2PtI_6 as the active absorber layer reaching power conversion efficiencies of up to 13.88% when paired with acceptable electron and hole transport materials. Furthermore, simulations of trials using the SCAPS-1D platform have predicted better performance. A simulated device configuration including FTO/SnO_2/Cs_2PtI_6/MoO_3 displayed a PCE of 23.52%, an V_{oc} of 1.118 V, a J_{sc} of 26.95 mA/cm^2, and a FF of 78.08% [14, 15]. The results highlight the great potential of Cs_2PtI_6 as a lead-free, high-performance alternative for next-generation perovskite solar cells.

Perovskite solar cells (PSCs) have shown a great deal of interest in carbon nanotubes (CNTs) because of their better charge transport capabilities and structural versatility. They have been effectively incorporated into a variety of device topologies, serving as charge-selective electrodes, dopant additives, interface modifiers, and complete hole transport layers (HTLs). PSCs' operational lifespan is increased by the inherent chemical and mechanical stability of CNT-based materials, overcoming a major barrier to their commercialisation [16]. High electrical conductivity, huge aspect ratios, and variable optical transparency make carbon nanotubes (CNTs) appealing for solar uses. With up to 92% optical transparency and a low sheet resistance of 85 Ω/sq [17], enhanced SWCNT films beat traditional transparent conductors, including ITO. When utilised as HTLs, SWCNTs have also been proven to increase moisture resistance and PCEs; under humid settings, this value ranges up to 19.98%. These characteristics draw attention to how well CNTs might enable the creation of dependable, versatile, and efficient perovskite-based solar systems [18].

Particularly in its mixed-valence form (CeO_2) and trivalent form (Ce_2O_3), cerium oxide (CeO_x) has shown promise for incorporation into PSCs. CeO_x's favourable physicochemical characteristics make it ideal for use as an interfacial moderator or ETL. Its broad bandgap, variable work function, great optical transparency, and well-matched energy levels with a variety of perovskite absorbers are among its main features. These properties not only promote effective electron extraction but also function as a barrier to hole transport, therefore reducing charge recombination losses at important interfaces and so improving general device performance. Apart from improving charge selectivity, CeO_x also improves device lifetime by protecting the perovskite layer from environmental degradation, mainly from moisture and oxygen exposure. Effective CeO_x integration into PSC designs has been established by recent experimental investigations to provide improved charge carrier dynamics and enhanced solar performance [19-21]. One study found a short-circuit current density J_{sc} of 30.79 mA/cm², a V_{oc} of 0.92 V, and a PCE of 17.77% [18] when cerium oxide (CeO_2) was the ETL [22].

EXPERIMENTAL

Proposed Design

As shown in Figure 1, the suggested solar cell design uses a typical planar heterojunction architecture, carefully modified to enhance charge carrier dynamics and light absorption. Comprising indium tin oxide (ITO), a transparent conductive material that effectively lets light flow through and acts as the anode, the front contact is the ETL is cerium oxide (Ce_2O_3) straight under the ITO. Ce_2O_3 not only promotes selective electron extraction but also helps control interfacial recombination losses using its broad bandgap, outstanding thermal stability, and high electron mobility. Made of all-inorganic caesium platinum iodide (Cs_2PtI_6), a lead-free perovskite-inspired material identified for its appropriate bandgap, excellent light absorption, and enhanced environmental stability relative to conventional hybrid organic–inorganic perovskites. Using their remarkable electrical conductivity, chemical durability, and low-temperature manufacturing compatibility, a layer of carbon nanotubes (CNTs) is included into the design to guarantee efficient hole collecting. Ultimately, the great electrical conductivity and reflectivity of a gold

(Au) rear contact help to further increase device efficiency using better photon cycling. Key problems like material toxicity, stability under running circumstances, and interfacial charge transfer are addressed by this well-crafted multilayer structure. SCAPS-1D was used for device simulations; input values were from past work [23, 24]. Each layer's thickness was methodically adjusted using batch simulations to maximise general performance, therefore enabling an iterative process to identify the most effective device design.

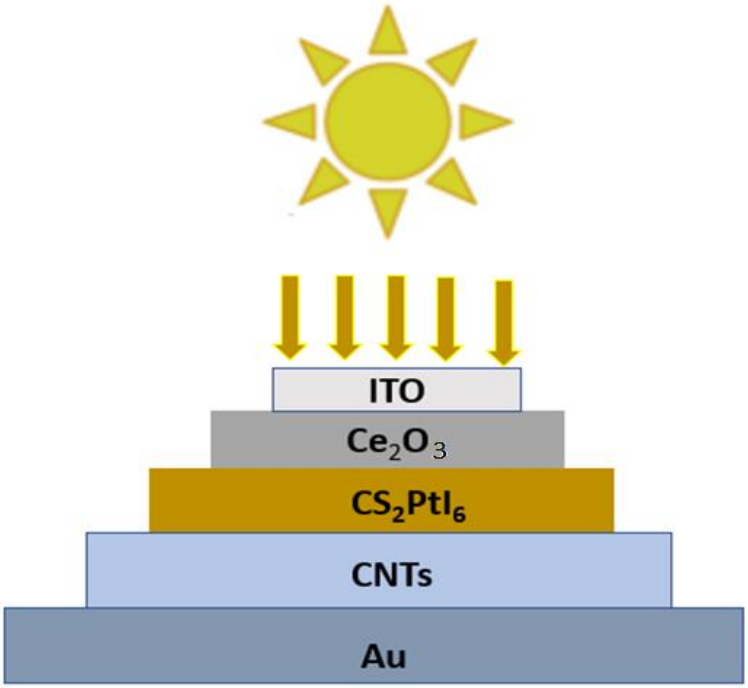

Figure 1. Cross-sectional schematic of a proposed solar cell.

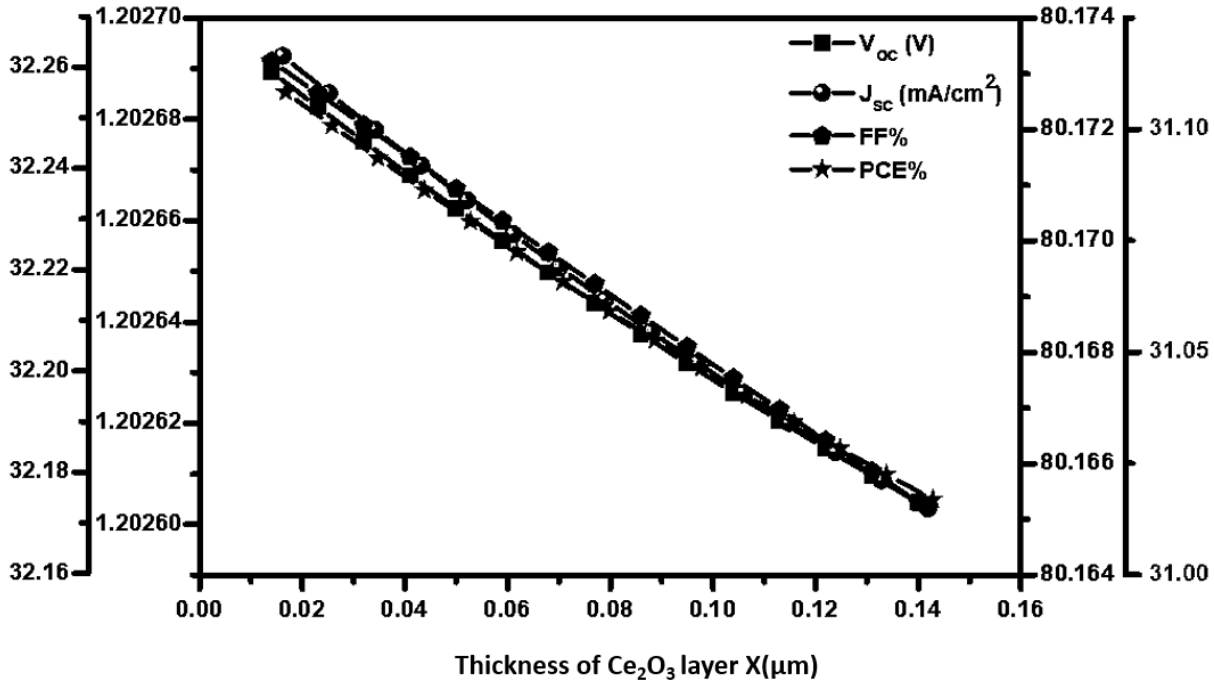

Figure 2. The influence of the Ce_2O_3 layer thickness on the performance metrics of proposed cells.

RESULTS AND DISCUSSION

Figure 2 depicts the effect of Ce_2O_3 layer thickness on the photovoltaic performance of the ITO/Ce_2O_3/Cs_2PtI_6/CNTs/Au solar cell, as modelled in SCAPS-1D. As the thickness of Ce_2O_3 grows from 0.01 µm to 0.15 µm, a progressive reduction is seen in all principal output parameters, including V_{oc}, J_{sc}, FF, and PCE. V_{oc} diminishes from roughly 1.20270 V to 1.20260 V, J_{sc} falls from 32.26 to 32.16 mA/cm^2, FF marginally reduces from 80.174% to 80.164%, and PCE declines from 31.10% to 31.00%. This development underscores the essential significance of ETL thickness in device optimisation. Thinner Ce_2O_3 layers provide enhanced charge extraction and reduce series resistance, however, larger layers may obstruct carrier movement and elevate recombination losses. The results indicate that optimising the thickness of Ce_2O_3 is crucial for enhancing device performance and achieving optimum electron selectivity in lead-free perovskite-inspired solar cells.

The current–voltage (J–V) curve of the suggested solar cell, simulated using SCAPS-1D under standard test conditions, illustrates the enhanced performance of this lead-free, carbon-nanotube-based device, figure 3. The obtained photovoltaic parameters consist of a V_{oc} of 1.20265 V, a J_{sc} of 32.22 mA/cm$_2$, a FF of 80.17%, and a power conversion efficiency (PCE) of 31.07%. The elevated V_{oc} indicates significant inherent potential and little recombination losses, while the augmented J_{sc} suggests effective photon absorption and carrier collection, primarily enabled by the direct bandgap and high absorption coefficient of Cs_2PtI_6. The fill factor over 80% signifies efficient charge extraction, due to the conductive and stable properties of the CNTs layer used as the hole transport medium. The continuous curve of the J–V profile further confirms the superior diode performance and the optimally designed device. The results highlight the essential role of carbon nanotubes in improving electrical conductivity and moisture resistance, therefore enabling their integration into stable, high-efficiency, and environmentally sustainable perovskite-inspired photovoltaic systems.

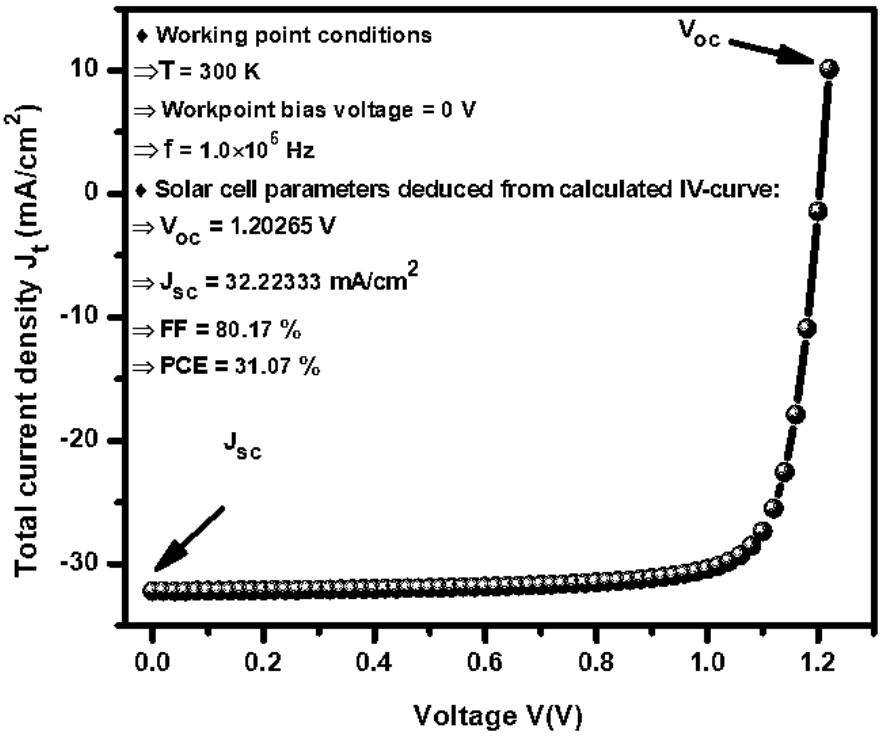

Figure 3. Current-voltage characteristics for the optimized solar cell.

Figure 4 provides a detailed examination of the effect of the Cs_2PtI_6 absorber layer thickness, spanning from around 1.2 µm to 2.3 µm, on the performance parameters of the simulated solar cell. The primary photovoltaic metrics being examined are the V_{oc}, J_{sc}, FF, and overall PCE. An increase in the thickness of the Cs_2PtI_6 layer correlates with a significant boost in J_{sc}. This enhancement is ascribed to increased optical absorption in the thicker absorber, facilitating the conversion of a higher number of incoming photons into charge carriers. The augmented photogeneration improves current output, making thicker layers more efficient at light absorption. Nonetheless, this advantage incurs some cost. As the layer thickness increases, both V_{oc} and FF start to decrease. The decrease in V_{oc} is probably due to heightened bulk recombination losses, whereby charge carriers produced deeper inside the absorber layer possess a lower likelihood of reaching the corresponding contacts before recombination. Likewise, fill factor diminishes owing to increased series resistance and a less effective charge extraction mechanism, which are prevalent in devices characterised by extended carrier transport pathways. The recombination and resistive losses together diminish the electrical quality of the device, particularly at increased thicknesses.

The performance of the PCE about absorber thickness reveals a clear balance between beneficial and limiting factors. At first, increasing the thickness of the Cs_2PtI_6 absorber layer leads to a noticeable boost in PCE, primarily due to the rise in J_{sc} as more light is absorbed. However, beyond an optimal point identified in this study as around 1.5 to 1.6 µm the gains in J_{sc} begin to level off, while the V_{oc} and FF start to decline. Higher recombination rates and more resistive losses from longer paths for charge carrier transport most likely explain this decline. As such, each additional thickness reduces the efficiency returns. This tendency emphasises the need of precisely controlling absorber layer thickness in solar cells inspired by perovskite. Strong light absorption is enabled by a Cs_2PtI_6 thickness that reaches an efficient equilibrium, thereby controlling recombination and transport losses. These revelations highlight the importance of exact thickness engineering to fully realise lead-free, ecologically friendly solar systems.

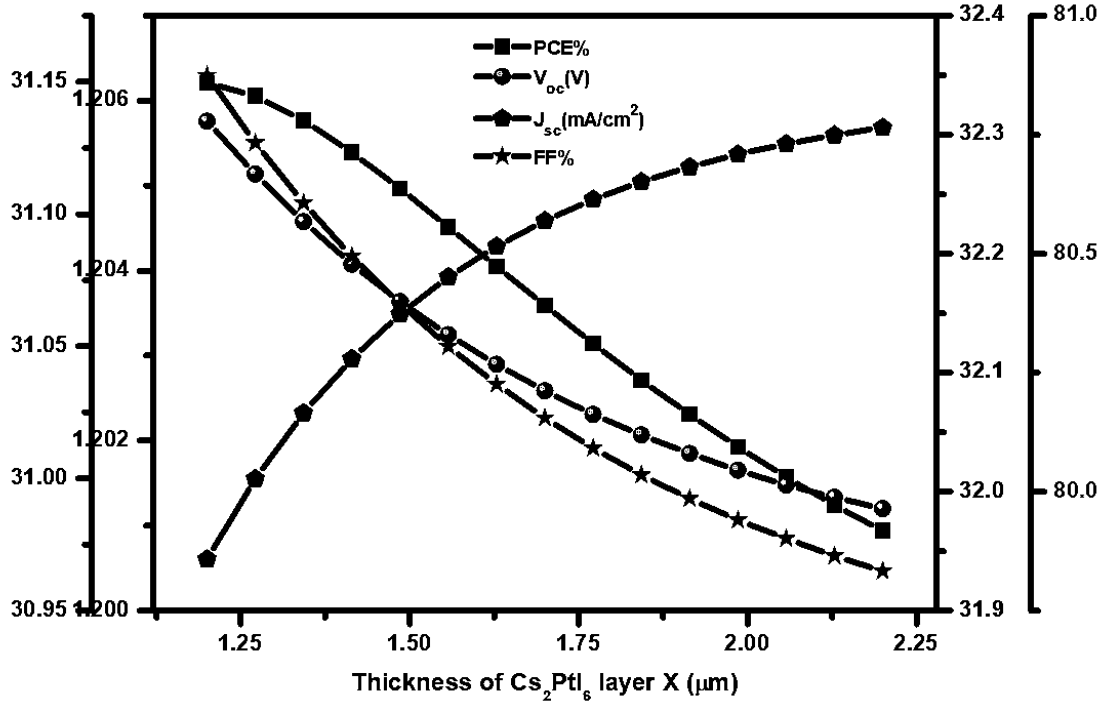

Figure 4. The influence of Cs_2PtI_6 layer thickness on the performance metrics of the proposed cell.

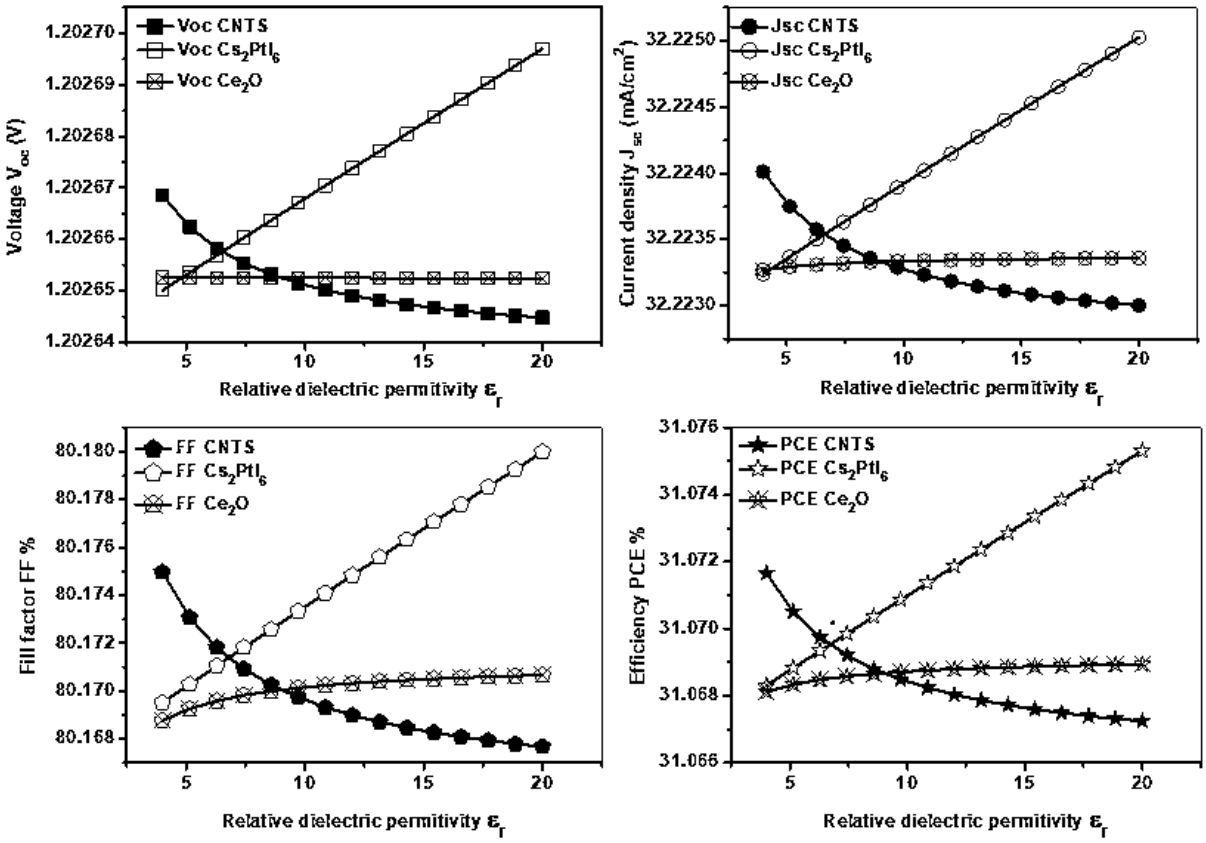

Figure 5. The influence of the relative permittivity of structural layers on performance attributes.

The relative dielectric permittivity (ϵF) of three significant layers CNTs (hole transport layer), Cs_2PtI_6 (absorber), and Ce_2O_3 (electron transport layer) affects the photovoltaic performance of the simulated solar cell, shown in figure 5. The image shows four subplots showing the trends in open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (PCE), as the dielectric constant spans 4 to 20. Of these layers, the Cs_2PtI_6 absorber has the biggest influence. All four performance criteria become much better as its ϵ_r rises. Better dielectric screening is probably responsible for this increase, as it lowers Coulombic attraction between photo-generated electron-hole pairs, hence enabling exciton dissociation and enhancing charge transfer. Together, the higher carrier mobility and lower recombination increase the electrical output of the cell. By contrast, variations in the dielectric constant of the CNTs and Ce_2O_3 layers show no effect or a little drop in performance. Higher values in these layers may induce dielectric losses or subtly change the internal electric field distribution, therefore influencing either carrier mobility or recombining rates. The results highlight generally the great relevance of optimising the dielectric characteristics of the absorber layer especially Cs_2PtI_6 to increase light absorption, enable efficient carrier separation, and boost charge collecting. Based on perovskite-inspired materials, this work provides insightful analysis of how dielectric engineering may be deliberately used to develop stable, lead-free, and high-efficiency solar cells.

CONCLUSION

This work emphasises the critical part the Ce_2O_3 electron transport layer plays in allowing lead-free solar cells with excellent efficiency. Ce_2O_3 promotes effective electron extraction, reduces recombination losses, and helps to provide general device stability using its favourable band alignment, broad bandgap, and strong dielectric characteristics. Not less significant is the effect of the Cs_2PtI_6 absorber layer, whose performance is very sensitive to both its thickness and relative dielectric permittivity (ϵ_r). Between increased light absorption and decreased charge transport and recombination losses, an optimum thickness of 1.5–1.6 μm offers the best balance. By helping exciton dissociation and improving carrier mobility, raising the ϵ_r of Cs_2PtI_6 also greatly enhances important photovoltaic properties. Variations in the dielectric constant of the CNTs and Ce_2O_3 layers, on the other hand, indicated either insignificant or somewhat negative impacts, most likely from changes in the internal electric field distribution. These findings underline generally the need of combining Ce_2O_3 as an effective ETL with dielectric and structural

tailoring of the absorber layer. Stable, sustainable, and high-performance solar cell technologies find their path thanks to this combined strategy.

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