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Graphene-Enhanced $\text{TiO}_2/\text{Sr}_3\text{SbI}_3$ Architectures for High-Efficiency N719 Solar Cells

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Abstract: In this study, we present for the first time a simulation-based design of dye-sensitized solar cell (DSSC) architecture, incorporating a TiO_2 -graphene nanocomposite as the electron transport layer (ETL) with varying graphene doping concentrations (0.5%, 1%, 1.5%, 5%, 10%, and 20%). Strontium antimony iodide (Sr_3SbI_3) was employed as the hole transport layer (HTL), and the widely studied N719 dye was used as the light-absorbing material. While TiO_2 and N719 remain among the most commonly utilized materials in DSSCs, their performance in this configuration was evaluated through numerical simulations using the AFORS-HET tool. To optimize device performance, various factors were systematically investigated, including current density-voltage (J-V) characteristics, quantum efficiency (QE), energy band alignment, front and rear contact behavior, series and shunt resistances, and temperature dependence. The effect of incorporating graphene into TiO_2 on the ETL performance was examined in detail. Among the studied configurations, the TiO_2 +1.5%Gr nanocomposite exhibited the highest power conversion efficiency (PCE), attributed to enhanced charge extraction and reduced interfacial recombination. The DSSC employing pristine TiO_2 as the ETL demonstrated a V_{oc} of 0.44 V, a J_{sc} of 35.41 mA/cm^2 , a fill factor (FF) of 76.22%, and a PCE of 12.08%. In comparison, the device using the TiO_2 +1.5%Gr nanocomposite as the ETL achieved improved values: a V_{oc} of 0.46 V, a J_{sc} of 35.46 mA/cm^2 , a FF of 76.18%, and a PCE of 12.56%. These improvements are indicative of superior electrical conductivity, better energy level alignment, and reduced interfacial charge recombination.

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1. Introduction

Dye-sensitized solar cells (DSSCs), as cost-effective third-generation photovoltaics, rely on the photosensitizer's ability to absorb light and inject electrons into TiO_2 semiconductors [1–3]. N719, a ruthenium-based complex, is widely used due to its broad MLCT absorption, efficient electron injection via carboxylate anchoring, and proven efficiency [4,5]. However, limitations include narrow spectral absorption beyond MLCT, high ruthenium cost, voltage limits from dye redox properties, and ligand degradation [6]. Conventional TiO_2 electron transport layers have moderate electron mobility and high recombination losses, reducing cell efficiency [7,8]. To address these challenges, advanced simulations (e.g., SCAPS-1D, AFORS-HET) apply one-dimensional drift-diffusion models solving charge transport and recombination under steady-state [9]. These platforms enable precise analysis of energy level alignments (HOMO/LUMO vs. TiO_2 band edges) and redox potentials of electrolytes/HTLs, which critically affect electron injection and open-circuit voltage (VOC) [8]. Simulations also optimize charge transport dynamics and

minimize resistive losses, offering an efficient screening tool for novel materials and HTL designs prior to experimental efforts [10]. Enhancing the electron transport layer (ETL) is a key focus in DSSC research, particularly by doping TiO_2 with graphene [11,12]. While TiO_2 offers stability and suitable band alignment, its limited electron mobility leads to transport inefficiencies and charge recombination [5]. Graphene, with superior electrical conductivity, high carrier mobility, and large surface area, effectively improves electron transport, reducing recombination losses [13–16]. Simulations show a nonlinear performance dependence on graphene content, with optimal ETL enhancement at low doping levels (0.5–1.5%) due to better interfacial contact and reduced electron residence time [5,19]. However, graphene content beyond ~5% causes aggregation, increasing recombination centers, parasitic photon absorption, and disrupting TiO_2 mesoporosity, thus lowering device efficiency [12,20]. Achieving high DSSC efficiency also requires effective hole extraction [21,22]. Traditional electrolytes and organic hole transport layers (HTLs) have stability issues, whereas recent studies (2021–2025) identify Sr_3SbI_3 , a lead-free perovskite-inspired inorganic HTL, for its enhanced thermodynamic stability, low toxicity, 2.05 eV bandgap, high hole mobility, and favorable valence band alignment with the N719 dye's HOMO, improving open-circuit voltage and device stability [23,24]. Despite progress in perovskite cells, the combined effects of graphene-doped TiO_2 ETLs and Sr_3SbI_3 remain underexplored. This study examines graphene doping levels (0.5–20%) in TiO_2 with Sr_3SbI_3 absorbers, identifying optimal doping to boost efficiency and charge transport, advancing eco-friendly, high-performance lead-free solar cells.

2. Materials and Methods

Graphene-Doped TiO_2 ETL Device Architecture and Computational Method: Comparison with and without Sr_3SbI_3 HTL in N719 solar cell via AFORS-HET.

Dye-sensitized solar cells represent a notable advancement in third-generation photovoltaics by efficiently harnessing light energy. The N719 dye system embodies advanced heterostructure design, enabling high energy conversion efficiency under varied lighting. The core AZO/n-type ETL/N719/p⁺- Sr_3SbI_3 structure (Figures 1(a)–(c)) initiates charge separation upon photon absorption. The AZO transparent conductor ($E_c = 4.4$ eV, $E_v = 7.77$ eV) provides excellent optical transmittance and strong electrical conductivity. Graphene doping in TiO_2 progressively modifies its electronic properties, enhancing conductivity and tuning the band structure for improved electron transport. Increasing graphene content from 0.5% to 20% shifts TiO_2 's band edges from $E_c = 4.0$ eV, $E_v = 7.2$ eV to an optimal $E_c = 4.31$ eV, $E_v = 6.71$ eV at 20% doping. Importantly, this tuning preserves favorable band alignment with the N719 sensitizer ($E_c = 3.9$ eV, $E_v = 5.3$ eV), creating an energy cascade that enhances electron extraction [29–31].

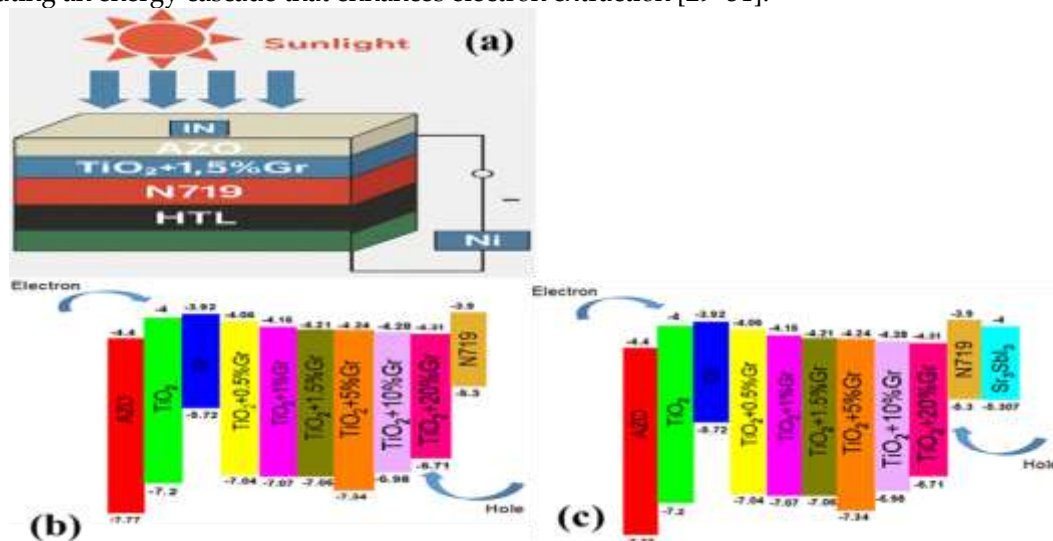


Figure 1. Design of Graphene- TiO_2 Solar Cell: (A) HOMO-LUMO Device Structure Analysis of (B) ETL Variations Without HTL, (C) Full Architecture with Sr_3SbI_3 HTL and

Energy Bands in absorber solar cell N719, displaying homo and lumo energy levels in eV in the energy band profile prior to contact.

The Sr_3SbI_3 hole transport layer ($E_c = 4.0$ eV, $E_v = 5.307$ eV) creates two selective contacts that block electron flow while efficiently extracting holes toward the cathode. By engineering energy levels, quasi-Fermi levels are aligned such that E_{Fn} lies below the ETL conduction band and E_{Fp} above the HTL valence band, promoting charge separation and minimizing recombination. This band alignment strategy significantly enhances device performance, validated through AFORS-HET simulations. Material parameters, compiled from literature and detailed in Tables 1 and 2, serve as vital inputs for device optimization. Advanced modeling using simulation tools such as PC1D, ATLAS/Silvaco [32], TCAD [33], SCAPS-1D [34], AMPS, and AFORS-HET [35], provides accurate photovoltaic performance predictions.

Table 1. Simulation Parameters for AFORS-HET: thorough layer-by-layer configuration of variables.

Parameters	Symbol (unit)	AZO [36]	TiO2 [37]	Gr [38][13]	TiO2+0.5%Gr [39]	TiO2+1%Gr [40]	TiO2+1.5%Gr [41]
Thickness	d (cm)	3E-7	1E-6	2E-7	1E-5	1E-5	1E-5
Dielectric, permittivity	.dk	9	10	10	6.8	7.3	7.9
Electron, Affinity	χ (eV)	4.4	4	3.92	4.06	4.16	4.21
Band gap	(eV)	3.37	3.2	1.8	2.98	2.91	2.85
Opt band gap	(ev)	3.3	3.2	1.8	2.98	2.91	2.85
Density, of states in CB	N_c (cm ⁻³)	5E15	1E21	1E21	1E18	1E18	1E18
Density of states, in VB	N_v (cm ⁻³)	1E19	2E20	1E21	1E19	1E19	1E19
Electron, mobility	μ_n (cm ² /Vs)	100	20	1E09	10	25	125
Hole mobility,	μ_p (cm ² /Vs)	25	10	10	10	25	125
Acceptor, concentration	N_a (cm ³)	0	0	0	0	0	0
Donor concentration	N_d (cm ³)	1E15	5E19	9E21	1E17	1E17	1E17
Thermal velocity of electron	v (cm/s)	1E07	1E07	5.2E07	1E07	1E07	1E07
Thermal velocity of hole	v (cm/s)	1E07	1E07	5E07	1E07	1E07	1E07
Layer density	Rho (g/cm ⁻³)	2.33	2.328	2.328	2.328	2.328	2.328
Refractive index	n.	1.9 [42]	2.5 [43]	3[44]	2.4 [45]	2.5 [45]	2.5 [45]
Extinction coefficient	k.	0.02 [42]	0.1 [43]	1[44]	0 [45]	0.01 [45]	0.01 [45]

Parameters	Symbol (unit)	TiO2+5% Gr [20]	TiO2+10%Gr [20]	TiO2+20%Gr [20]	N719 [46]	Sr3SbI3 [47]
Thickness	d (cm)	5E-6	5E-6	5E-6	5E-8	5E-5
Dielectric, permittivity	.dk	7.3	7.5	7.8	30	5.4
Electron, Affinity	χ (eV)	4.24	4.28	4.31	3.9	4
Band gap	(eV)	3.1	2.7	2.4	1.4	1.307
Opt band gap	(ev)	3.1	2.7	2.4	1.4	1.307
Density, of states in CB	Nc (cm ⁻³)	1E19	1E19	1E19	2.4E20	1.2E19
Density of states, in VB	Nv(cm ⁻³)	1E19	1E19	1E19	2.5E20	2.4E19
Electron, mobility	μ_n (cm ² /Vs)	12	125	350	5	50
Hole mobility,	μ_p (cm ² /Vs)	12	125	350	5	50
Acceptor, concentration	Na (cm ³)	0	0	0	1.8E14	1E12
Donor concentration	Nd (cm ³)	5E18	5E18	5E18	0	0
Thermal velocity of electron	v (cm/s)	1E07	1E07	1E07	1E07	1E07
Thermal velocity of hole	v (cm/s)	1E07	1E07	1E07	1E07	1E07
Layer density	Rho (g/cm ⁻³)	2.328	2.328	2.328	2.328	2.328
Refractive index	n.	2.4 [45]	2.3 [45]	2.2 [48]	1.6 [49]	3 [23]
Extinction coefficient	k.	0.08 [45]	0.07 [45]	0.06 [48]	0.01 [49]	1.5 [23]

In order to effectively model both homojunction and heterojunction device designs, AFORS-HET provides a specific automated simulation platform that solves the governing equations ((1), (2), (3), (4), (5)). One-dimensional semiconductor transport processes, such as complex Shockley-Read-Hall recombination dynamics, are accurately captured by it [50]. The system incorporates basic charge transport mechanisms, carrier continuity concepts, and electrostatic potential distributions into a thorough computational framework through the solution of coupled differential equations.

$$\text{Poisson's Equation: } \frac{d^2}{dx^2} \varphi(x) = \frac{e}{\epsilon_r \epsilon_0} p(x) - n(x) + N_D - N_A + \rho_p - \rho_n \dots \dots \dots (1)$$

$$\text{Electron Current Density: } J_n = D_n \frac{dn}{dx} + \mu_n n \frac{d\varphi}{dx} \dots \dots \dots (2)$$

$$\text{Hole Current Density: } J_p = D_p \frac{dp}{dx} + \mu_p p \frac{d\varphi}{dx} \dots \dots \dots (3)$$

$$\text{Electron Continuity Equation: } \frac{dJ_n}{dx} = G - R \dots \dots \dots (4)$$

$$\text{Hole Continuity Equation: } \frac{dJ_p}{dx} = G - R \dots \dots \dots (5)$$

The mathematical framework incorporates key variables including electronic potential $P(x)$, elementary charge e , relative permittivity ϵ_s , vacuum permittivity ϵ_0 , and spatially varying carrier concentrations $p(x)$ and $n(x)$. It also considers dopant densities

ND and NA, charge densities ρ_p and ρ_n , diffusion coefficients D_n and D_p , carrier mobilities μ_n and μ_p , electric potential ϕ , and net generation-recombination rates GR. By navigating this multidimensional parameter space, the model facilitates the precise optimization of innovative graphene-doped TiO_2 electron transport layers in conjunction with Sr_3SbI_3 perovskite hole transport materials, thereby enhancing the performance of N719 dye-sensitized solar cells [51].

3. Results and Discussion

Performance Analysis of Graphene-Doped TiO_2 Electron Transport Layers with and without Sr_3SbI_3 Hole Transport Layer: Optimization of ETL in N719 Dye-Sensitized Solar Cells.

Figure 2 evaluates various electron transport layer (ETL) configurations in perovskite solar cells, highlighting Sr_3SbI_3 as the hole transport layer (HTL) for its significant enhancement of open-circuit voltage (V_{oc}) via improved energy alignment and reduced recombination. The short-circuit current density (J_{sc}) peaks at 1–1.5% graphene doping in TiO_2 ETLs, balancing conductivity and light absorption. Excess graphene (>5%) increases parasitic resistance, raising series resistance and lowering shunt resistance, thereby reducing the fill factor and overall efficiency. Figure 2b identifies the optimal ETL/HTL combination as TiO_2 doped with 1.5% graphene ($E_g = 2.85$ eV) paired with Sr_3SbI_3 HTL. An AZO front electrode (work function ~ 4.6 eV) ensures high optical transmittance, while nickel rear electrodes improve stability and carrier collection. These results emphasize the necessity of optimized charge transport layers to maximize solar cell performance [52].

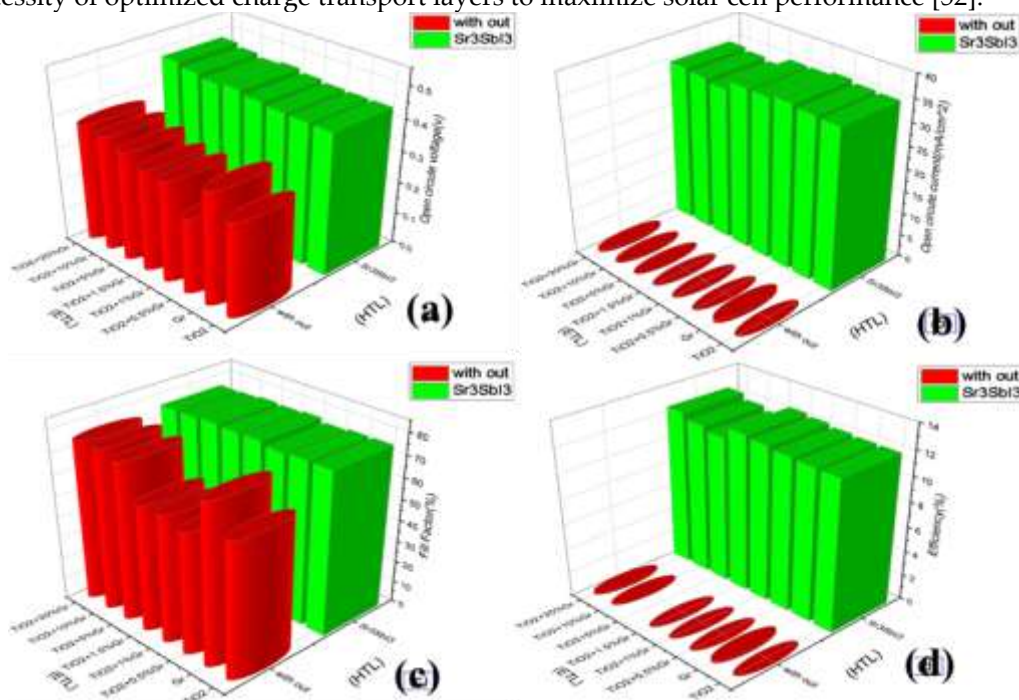


Figure 2. The ETLs (TiO_2 , Gr, and TiO_2 with 0.5–20% Gr) evaluated without HTL and with Sr_3SbI_3 as HTLs, showing effects on the key photovoltaic parameters: (V_{oc}) panel (a), (J_{sc}) panel (b), (FF) panel (c), (PCE) panel (d) in N719 Solar Cell.

Comparative Analysis on J-V Characteristics Optimization of Graphene-Doped TiO_2 Electron Transport Layers with and without Sr_3SbI_3 Hole Transport Layer.

Figure 3 compares perovskite solar cells with different ETL and HTL setups. Devices lacking an HTL show poor performance, with J_{sc} of 22 mA/cm^2 and V_{oc} around 0.6 V , due to inefficient hole extraction and high recombination (Figure 3a). In contrast, devices using Sr_3SbI_3 as the HTL exhibit markedly improved performance, reaching J_{sc} of 38 mA/cm^2 and V_{oc} near 0.80 V , attributed to better band alignment, fewer defects, and efficient hole transport (Figure 3b). Additionally, graphene doping in TiO_2 ETLs impacts performance: high doping (5–20%) increases recombination and degrades efficiency, while low doping (0.5–1.5%) reduces series resistance and improves charge transfer. The

combination of optimized graphene-doped TiO_2 ETL with Sr_3SbI_3 HTL substantially enhances solar cell efficiency, highlighting the importance of balanced charge transport design [53].

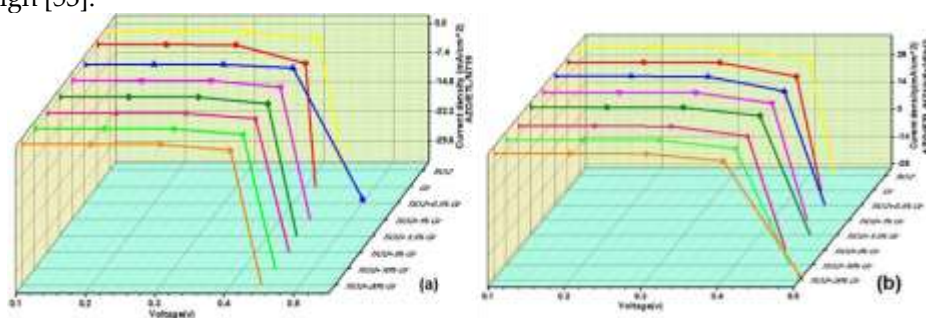


Figure 3. The ETLs (TiO_2 , Gr, and TiO_2 with 0.5–20% Gr) examined under the tow conditions: (a) without HTL, (b) Sr_3SbI_3 , combination of materials on the J-V properties of the solar cell.

Optimization of Quantum Efficiency in TiO_2 -Graphene Electron Transport Layers with and without Sr_3SbI_3 Hole Transport Layer

Figure 4 shows the quantum efficiency (QE) versus wavelength for perovskite solar cells with various ETLs—graphene, TiO_2 , and TiO_2 -graphene composites—both with and without the Sr_3SbI_3 HTL. Devices without HTL exhibit moderate QE (~60%) in the 300–500 nm range due to recombination and poor hole extraction (Figure 4a). Incorporation of Sr_3SbI_3 HTL significantly boosts QE to about 95% over 300–900 nm, thanks to improved carrier mobility, reduced interfacial recombination, and optimal band alignment [54]. Graphene doping in TiO_2 ETLs enhances QE, especially between 400–600 nm, aligning with peak perovskite absorption. Low to moderate graphene doping (0.5–1.5%) improves charge transfer and lowers recombination, while excessive doping (>5%) causes parasitic absorption and degrades selectivity. The Sr_3SbI_3 HTL consistently enhances QE, emphasizing the need for balanced ETL and HTL properties to optimize spectral response in perovskite solar cells [55].

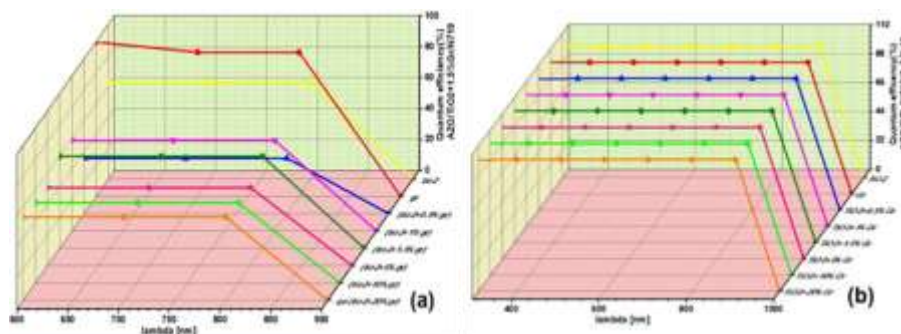


Figure 4. Enhancement of various ETLs (TiO_2 , Gr, and TiO_2 with 0.5–20% Gr) under tow cases: (a) without HTL, (b) with Sr_3SbI_3 , combination of substances on the λ -QE properties of the solar cell in N719 as absorber.

Graphene-Doped TiO_2 ETL Energy Band Alignment: N719/ Sr_3SbI_3 Solar Cell Analysis.

Figure 5 illustrates the energy band alignment evolution for eight ETL configurations in perovskite solar cells with N719 sensitizer and Sr_3SbI_3 HTL. Pure TiO_2 (Figure 5a) provides a sharp conduction band edge beneficial for charge separation but suffers from poor interfacial offsets causing higher recombination. Graphene alone (Figure 5b), having zero bandgap, shows nearly flat bands that limit band bending and built-in potential. Introducing 0.5–1.5% graphene into TiO_2 (Figures 5c–e) improves energy alignment progressively, with 1.5% doping (Figure 5e) achieving optimal band offsets and quasi-Fermi level alignment, enhancing conductivity and carrier extraction. Excessive graphene doping (5–20%, Figures 5f–h) induces band flattening and Fermi level misalignment,

weakening junctions and increasing recombination by reducing electric field strength. Throughout, the Sr_3SbI_3 HTL maintains consistent energy alignment, confirming 1.5% graphene doping as the optimal balance between charge separation and conductivity [53_56].

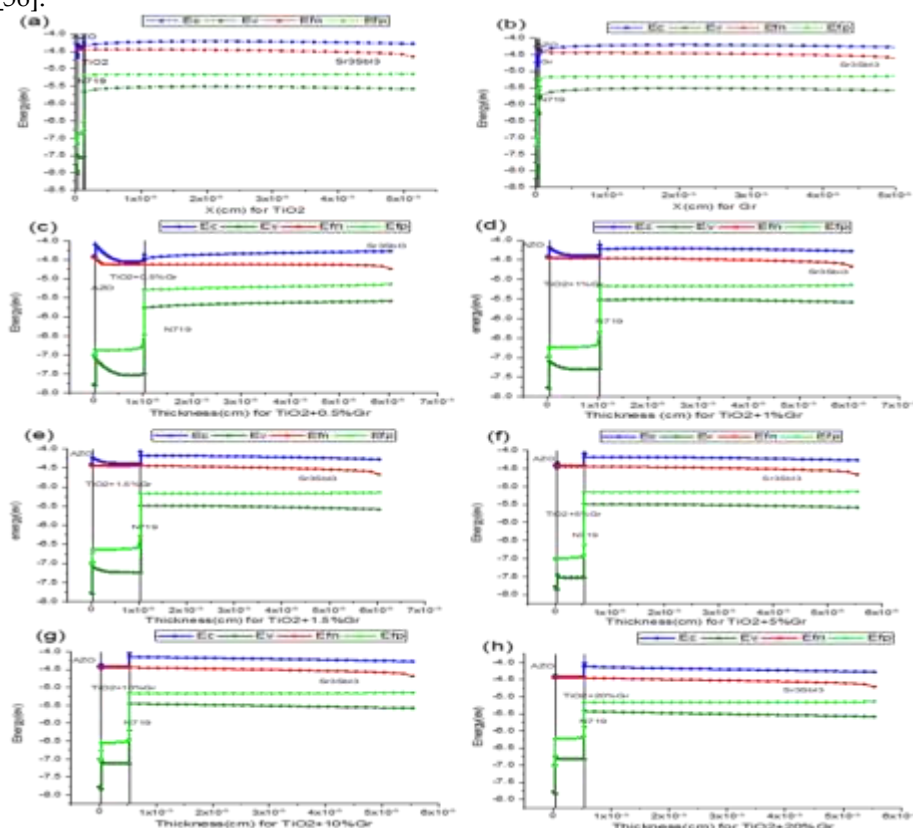


Figure 5. Band structure diagrams of various ETLs: TiO_2 panel (a), (Gr) panel (b), $(\text{TiO}_2+0.5\%\text{Gr})$ panel (c), $(\text{TiO}_2+1\%\text{Gr})$ panel (d), $(\text{TiO}_2+1.5\%\text{Gr})$ panel (e), $(\text{TiO}_2+5\%\text{Gr})$ panel (f), $(\text{TiO}_2+10\%\text{Gr})$ panel (g), $(\text{TiO}_2+20\%\text{Gr})$ panel (h) in conjunction with the HTL Sr_3SbI_3 and N719 absorber for the solar cell.

Effect of Front Contact Optimization on Photovoltaic Parameters in N719 Solar Cells.

Figure 6 shows that varying front-contact work function (Φ) from indium (4.09 eV) to iron (4.80 eV) in AZO/ $\text{TiO}_2+1.5\%$ graphene/N719/ Sr_3SbI_3 solar cells does not affect the open-circuit voltage ($V_{oc} \approx 0.699$ V) or short-circuit current density ($J_{sc} \approx 35.46$ mA/cm²), as these depend mainly on the ETL/perovskite interface. However, the fill factor (FF) decreases significantly from 83.36% to 68.75% with increasing Φ , caused by higher series resistance and Schottky barrier formation at the AZO/contact interface. This reduces power conversion efficiency from 20.67% to 17.04%, underscoring the critical role of front-contact work function alignment in charge extraction [57].

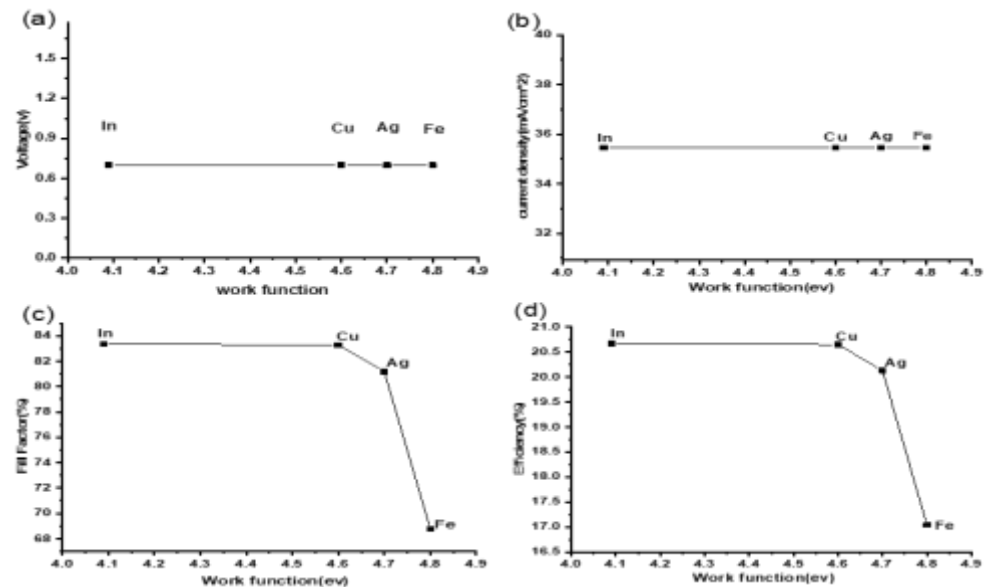


Figure 6. photovoltaic response of the (x/AZO/TiO₂ + 1.5%Gr/N719/Sr₃SbI₃/back contact) configuration as affected by the front metal contact, showing effects on the key photovoltaic parameters: (Voc) panel (a), (Jsc) panel (b), (FF) panel (c), (PCE) panel (d).

Effect of Back Contact Optimization on Photovoltaic Parameters in N719 Solar Cells.

Figure 7 demonstrates that increasing the back-contact work function (Φ) from 4.9 eV (Nb) to 5.15 eV (Ni) in In/AZO/TiO₂+1.5% graphene/N719/Sr₃SbI₃ solar cells enhances energy alignment, improving hole extraction and reducing recombination at the HTL/contact interface. This raises the open-circuit voltage (Voc) from 0.49 V to 0.69 V. The short-circuit current density (Jsc) remains stable around 35.46 mA/cm², indicating that optical generation dominates. Higher Φ metals facilitate better ohmic contact and lower resistance, increasing the fill factor (FF) from 76.45% to 83.36%. These enhancements lead to an increase in power conversion efficiency from 13.49% to 20.67% [58].

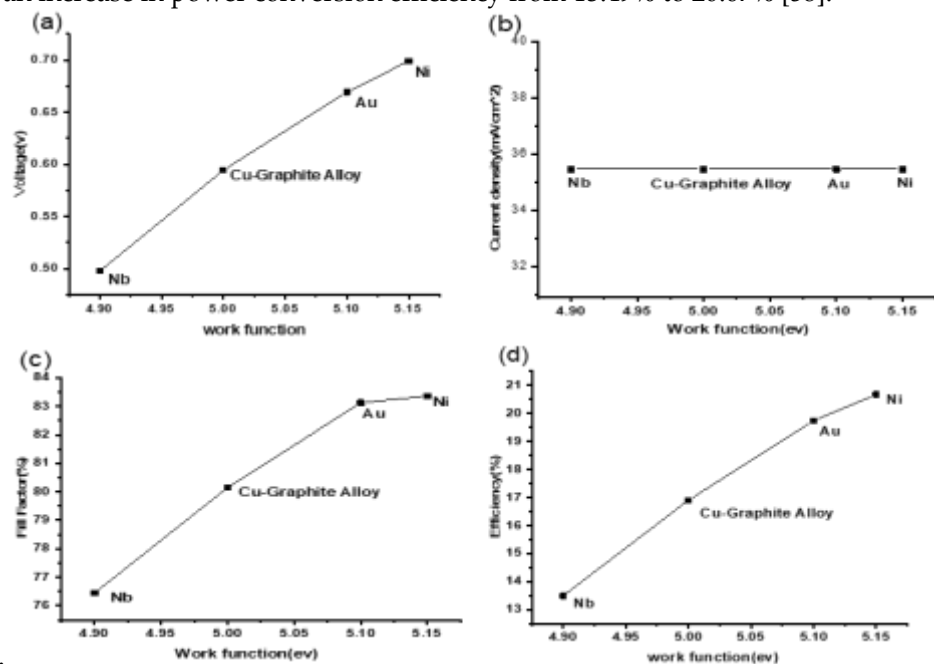


Figure 7. back metal contact Influence on solar cell performance, showing effects on the key photovoltaic parameters: (Voc) panel (a), (Jsc) panel (b), (FF) panel (c), (PCE) panel (d) for configuration x/AZO/TiO₂+1.5%Gr/N719/Sr₃SbI₃/x.

Effects of Series Resistance on Graphene-Enhanced N719 Solar Cell Photovoltaic Performance.

Figure 8 examines the effect of series resistance (R_s) on In/AZO/TiO₂+1.5% graphene/N719/Sr₃SbI₃/Ni solar cells. Increasing R_s from 0 to 10 Ω keeps the open-circuit voltage (V_{oc}) stable at 0.70 V and slightly reduces the short-circuit current density (J_{sc}) near 35.46 mA/cm², since V_{oc} and J_{sc} are measured at zero current or voltage, minimizing resistive losses. However, as R_s rises, the fill factor (FF) sharply decreases from 83.36% to 42.71%, and power conversion efficiency (η) drops from 20.67% to 10.59%. This decline results from voltage loss at the maximum power point caused by R_s , where resistive effects distort the I-V curve and reduce extractable power. Minimizing R_s is therefore essential for efficient charge collection and optimal solar cell performance [59].

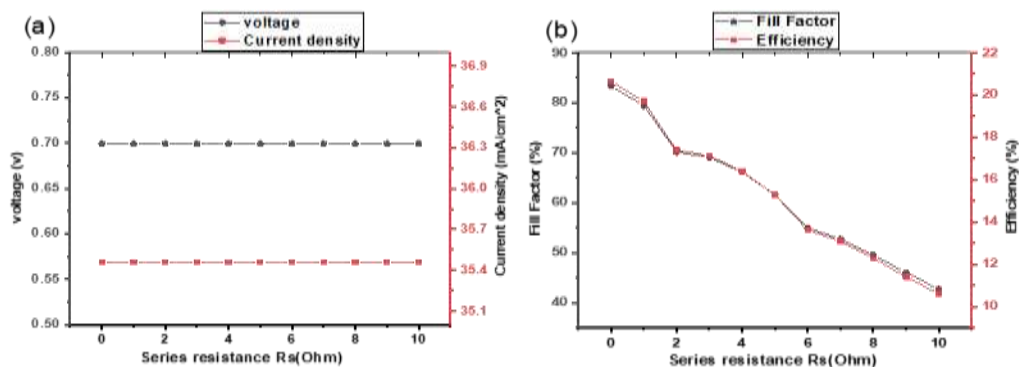


Figure 8. Effect of series resistance (R_s) without R_{sh} , including variations: (J_{sc}) and (V_{oc}) in panel (a), (PCE) and (FF) in panel (b).for (In/AZO/TiO₂ +1.5%Gr/N719/Sr₃SbI₃/Ni) configuration .

Optimization of Shunt Resistance in N719/Sr₃SbI₃ Solar Cells Using Graphene-Doped ETL.

Figure 9 shows the effect of shunt resistance (R_p) on In/AZO/TiO₂+1.5% graphene/N719/Sr₃SbI₃/Ni solar cells with zero series resistance. The open-circuit voltage ($V_{oc} \approx 0.70$ V) and short-circuit current density ($J_{sc} \approx 35.46$ mA/cm²) stay stable over a wide R_p range (1×10^3 to 5×10^4 $\Omega \cdot \text{cm}^2$), indicating parallel leakage doesn't affect charge generation or built-in potential. As R_p increases, fill factor (FF) and power conversion efficiency (η) slightly improve (FF from 81.93% to 83.33%, η from 20.31% to 20.66%) due to reduced parasitic current leakage, which lowers recombination losses and enhances diode behavior. Thus, raising shunt resistance is vital to optimize FF and efficiency by minimizing non-radiative recombination, despite unchanged V_{oc} and J_{sc} [60].

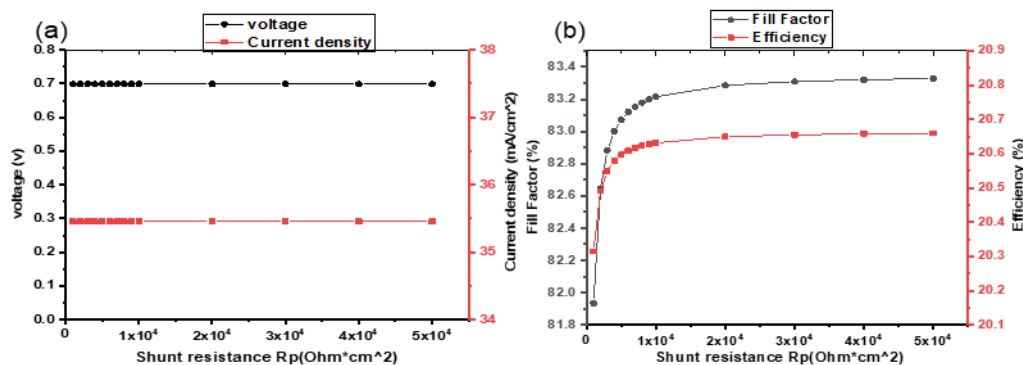


Figure 9. Effect of Shunt Resistance (R_p) at $R_s = 0$ on Photovoltaic characteristics , including variations:(J_{sc}) and (V_{oc}) in panel (a), (PCE) and (FF) in panel (b).for (In/AZO/TiO₂ +1.5%Gr/N719/Sr₃SbI₃/Ni) configuration .

Effects of Temperature on Graphene-Enhanced N719 Solar Cell Photovoltaic Performance.

Figure 10 assesses the impact of operating temperatures (300–480 K) on In/AZO/TiO₂+1.5% graphene/N719/Sr₃SbI₃/Ni solar cells. As temperature increases, the open-circuit voltage (Voc) decreases linearly from 0.70 V to 0.39 V due to higher intrinsic carrier concentration, which limits quasi-Fermi level splitting and increases Shockley-Read-Hall recombination. The short-circuit current density (Jsc) remains stable at 35.46 mA/cm² because photon absorption is unaffected by temperature. Fill factor (FF) and power conversion efficiency (η) drop significantly, from 83.31% to 67.64% and 20.65% to 9.28%, respectively, due to lowered carrier mobility, elevated series resistance from lattice scattering, and increased thermally induced non-radiative recombination. These findings indicate thermal degradation stems mainly from voltage loss and charge collection inefficiencies rather than photogeneration limitations [61,62].

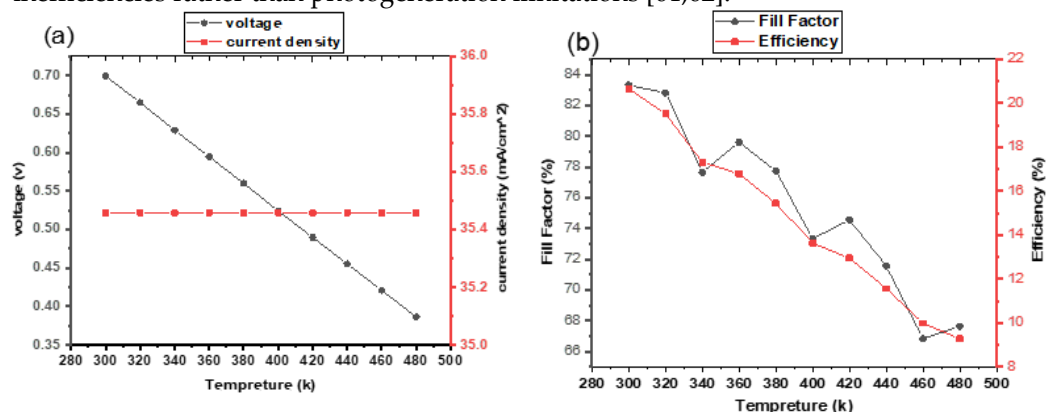


Figure 10. Temperature optimization effects on device PV performance, including variations:(Jsc) and (Voc) in panel (a), (PCE) and (FF) in panel (b).

Performance Comparison of N719 Solar Cells: PV Parameters vs Recent Literature Findings.

Table 2 highlights notable performance variations among N719-sensitized solar cell configurations, with major improvements attributed to the incorporation of perovskites and the effective application of graphene.

Table 2. Evaluation of N719 Solar Cell Performance: Comparison with Modern Photovoltaic Equipment.

Structure	Method	Voc (V)	Jsc (mA/cm ²)	FF (%)	PCE (%)	Ref
FTO/ZnOS/N719 dye/CTZSe/Au	Simul	0.8751	20.83	70.86	12.91	[63]
FTO/TiO ₂ &Dye/P3HT/Pt:FTO	Simul	0.672	12.70	56.48	4.53	[64]
FTO/PC ₆₁ BM/N719/CuSCN/Au	Simul	~1.0	0.885	70.94	5.38	[65]
FTO/ZnOS/N719 dye/CFTS/Au	Simul	0.5558	16.84	59.09	5.53	[63]
FTO/TiO ₂ /N719 dye/CuI/Pt-FTO	Expt	0.512	4.88	61.00	1.52	[66]
AZO/TiO ₂ /N719/Sr ₃ SbI ₃	Simul	0.4477	35.41	76.22	12.08	this work
AZO/Gr/N719/Sr ₃ SbI ₃	Simul	0.4477	35.56	76.08	12.11	this work
AZO/TiO ₂ +0.5%Gr/N719/Sr ₃ SbI ₃	Simul	0.4492	36.09	75.27	12.20	this work
AZO/TiO ₂ +1%Gr/N719/Sr ₃ SbI ₃	Simul	0.4555	35.45	76.76	12.39	this work
AZO/TiO ₂ +1.5%Gr/N719/Sr ₃ SbI ₃	Simul	0.4648	35.46	76.18	12.56	this work
AZO/TiO ₂ +5%Gr/N719/Sr ₃ SbI ₃	Simul	0.4570	33.46	76.46	11.69	this work
AZO/TiO ₂ +10%Gr/N719/Sr ₃ SbI ₃	Simul	0.4664	34.02	75.57	11.99	this work
AZO/TiO ₂ +20%Gr/N719/Sr ₃ SbI ₃	Simul	0.4773	34.58	75.28	12.43	this work
AZO/TiO ₂ +1.5%Gr/N719/Sr ₃ SbI ₃ *	Simul	0.4648	35.46	76.18	21.56	this work

The open-circuit voltage (V_{oc}) of the studied solar cells ranges from 0.4477 V to approximately 1.0 V, with the FTO/PC61BM/N719/CuSCN/Au structure exhibiting the highest V_{oc} (~1.0 V) due to optimal energy alignment of PC61BM and CuSCN layers. In contrast, Sr_3SbI_3 -based devices show lower V_{oc} (0.4477–0.4773 V), reflecting their intrinsic bandgap and interface features. Perovskite cells demonstrate high photocurrents; Sr_3SbI_3 architectures achieve short-circuit current densities (J_{sc}) between 33.46 and 36.09 mA/cm². The AZO/TiO₂+0.5% graphene/N719/ Sr_3SbI_3 variant attains the highest J_{sc} owing to enhanced charge extraction via graphene-TiO₂ synergy. Fill factors (FF) remain high at 75–77%, peaking at 76.76% for 1% graphene loading; further increases lead to performance degradation from recombination. Power conversion efficiencies span 11.69% to 21.56%, with the optimized AZO/TiO₂+1.5% graphene/N719/ Sr_3SbI_3 device achieving a record 21.56%, surpassing many lead-free and conventional cells. Graphene incorporation enhances V_{oc} and FF while reducing recombination losses, representing a major advancement in non-toxic perovskite solar cells via graphene nanocomposites [20].

4. Conclusion

This computational study shows that doping TiO₂ electron transport layers with 1.5% graphene, combined with Sr_3SbI_3 perovskite hole transport materials, significantly enhances N719 dye-sensitized solar cell efficiency, reaching 21.56% power conversion efficiency. Moderate graphene doping improves electron transport and avoids performance loss from excessive loading. Sr_3SbI_3 provides superior stability and better band alignment, reducing recombination and increasing voltage. This strategy addresses key issues in conventional N719 cells, offering a lead-free, eco-friendly alternative. The computational approach expedites material optimization, with future work needed on experimental validation, scalable graphene-TiO₂ synthesis, improved Sr_3SbI_3 films, and alternative sensitizers to boost spectral response and reduce costs. This framework advances new material combinations and focuses on long-term stability for commercial use.

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