

Numerical optimization of a monolithic WSe₂/WS₂ tandem solar cell: achieving 21.94% efficiency via bandgap engineering in SCAPS-1D

S. AMEEN, M. SAJID, K. ALI *

Nano-optoelectronics Research Laboratory, Department of Physics, University of Agriculture Faisalabad, 38040, Pakistan

Single-junction solar cells are fundamentally limited by the Shockley-Queisser efficiency ceiling due to incomplete utilization of the solar spectrum. In this work, we propose and numerically optimize a monolithic tandem solar cell based entirely on tungsten diselenide (WSe₂) using SCAPS-1D simulation software. The top cell employs germanium-incorporated WSe₂ (WSe₂:Ge) as the wide-bandgap absorber ($E_g \approx 1.6$ eV), while the bottom cell uses pristine WSe₂ as the narrow-bandgap absorber ($E_g \approx 1.0$ eV). A Cu₂O hole transport layer and ZnO electron transport layer are used to facilitate charge extraction. Systematic optimization of absorber layer thicknesses yields current-matched operation ($J_{sc} = 18.53$ mA/cm²) at top and bottom cell thicknesses of 1.08 μ m and 1.62 μ m, respectively. The optimized monolithic tandem structure achieves an open-circuit voltage (V_{oc}) of 0.743 V, short-circuit current density (J_{sc}) of 43.18 mA/cm², fill factor (FF) of 84.82%, and a power conversion efficiency (PCE) of 21.94% under standard AM1.5G illumination. This efficiency surpasses previously reported single-junction WSe₂ solar cells and demonstrates the potential of same-material monolithic tandem architectures using earth-abundant, non-toxic transition metal dichalcogenides. The results provide a theoretical foundation for experimental realization of high-efficiency WSe₂-based tandem photovoltaics.

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1. Introduction

Solar energy is a clean, renewable, and cost-effective power source, making it a vital component of sustainable energy solutions [1, 2]. However, conventional single-junction solar cells suffer from limited efficiency due to their inability to fully absorb low-energy photons [3, 4]. To overcome this limitation, tandem solar cells comprising multiple stacked p-n junctions have emerged as a promising alternative, enabling broader spectral absorption and enhanced power conversion efficiency. Recent studies have demonstrated that tandem configurations can achieve efficiencies exceeding 26%, particularly when optimized with thin-film absorber layers such as tin sulfide (SnS) [5-7]. This type of solar cell consists of two or more sub-cells, each set up to take in different parts of the solar spectrum. Experiments have shown that thin-film technologies that use materials such as cadmium telluride (CdTe), amorphous silicon (a-Si) and copper indium gallium selenide (CIGS) can be useful for such tasks. Even so, indium, gallium and tellurium are both rare and harmful which makes large-scale use difficult [8].

However, materials made from kesterite-based compounds such as copper zinc tin sulfide (CZTS) and CZTSSe are more sustainable and easily available. Merging a SnS layer below CZTS/CZTSe absorbers has greatly lowered the number of carriers that are easily lost, increasing the efficiency of the solar cells. The focus of this study is to improve the performance of tandem solar

cells through clever materials and design, mainly by altering the bandgap and changing the structure of the solar cells [9]. It reaches its overall high efficiency of 26.21% when made with a 0.2 μ m-thick layer of CZTS (Cu₂ZnSnS₄) and a p-n tunnel junction structure. By adjusting the design and thickness of the junction, this configuration can help photovoltaic devices perform better [10]. Moving towards tandem solar cells is helping to develop advanced photovoltaic technologies that meet important requirements such as being cost-effective, non-toxic and sustainable. TFSCs made with innovative absorber materials can achieve great photoconversion efficiency thanks to improved ways of trapping light. Currently, thin-film solar panels built with CIGS and CdTe can perform almost as well as silicon-based solar panels. Unfortunately, using these materials is complicated by issues such as scarcity of certain elements, their effect on the environment and costly production. Research is done on alternative ways to make solar cells and link them in tandem to reduce these limits and keep the conversion efficiency high [11]. Among transition metal dichalcogenides (TMDCs) [12], molybdenum disulfide (MoS₂) and tungsten disulfide (WS₂) are especially sought after in solar energy due to their excellent optoelectronic and electrochemical properties. Researchers in the solar field are paying close attention to these materials because they have adjustable bandgaps, strong abilities to interact with light and are likely to use earth-quantified element in devices. The way the atomic components organize in

WSe₂ is key to allowing the WS₂-based structures to have their properties changed for better performance, with no effect on the durability of the material [13]. Recently, we have shown that swapping cadmium sulfide (CdS) windows in CdTe cells with WS₂ allows them to work just as well, but without including toxic cadmium. This development is important for creating photovoltaic devices that are better for the environment and more efficient [14].

The hexagonal system (space group P6₃/mmc) is how tungsten disulfide (WS₂) and tungsten diselenide (WSe₂) form crystals. This type of material is known for its lamellar form where layers are held together by weak van der Waals interactions. Due to this specific structure, the material can accept foreign atoms between its layers which makes it possible to modify its properties. WS₂ and WSe₂ do not conduct electricity until hit by heat, when they become able to conduct electricity. Because of their low internal bond strength and adjustable electron behavior, they are well-suited for various advanced optoelectronic devices such as solar cells [15]. These materials function as semiconductors. As the temperature goes up, the activation energies and conductivity for sulphide become 0.18 eV for selenide and 0.12 eV [16]. The advancement of thin-film photovoltaic technology currently confronts three primary challenges: (1) cost reduction in manufacturing processes, (2) improvement of device performance metrics, and (3) enhancement of power conversion efficiency. Among emerging solutions, nanostructured solar cell architectures - particularly dye-sensitized solar cells (DSSCs) - demonstrate substantial potential to address these challenges simultaneously. These nanoscale-engineered systems offer distinct advantages in both production economics and efficiency optimization, positioning them as transformative candidates for next-generation solar energy [17]. Current state-of-the-art photovoltaic systems employ multi-junction architectures designed to maximize photon absorption across the solar spectrum. By utilizing stacked p-n junctions with varying bandgaps, these systems efficiently capture both high-energy and low-energy photons through spectral splitting. Among existing solar technologies, thin-film photovoltaics have emerged as particularly promising candidates due to their combination of high conversion efficiency, low maintenance requirements, operational simplicity, and minimal environmental impact. The device architecture incorporates optically transparent tunnel junctions that electrically connect subcells while simultaneously reflecting unabsorbed photons from the upper cell back for secondary absorption, thereby minimizing thermalization losses and maximizing energy conversion [18]. In single-junction photovoltaic devices, the absorber layer's bandgap energy (E_g) fundamentally constrains the spectral utilization efficiency. Photons with energies below E_g cannot be absorbed due to the material's bandgap limitation, while supra-bandgap photons dissipate their excess energy through thermalization processes. In both cases, a significant portion of the incident solar spectrum fails to contribute effectively to electrical power generation, resulting in substantial energy losses that limit

the theoretical maximum efficiency of single-junction solar cells to approximately 33% under standard illumination conditions (Shockley-Queisser limit) [19, 20]. Tandem photovoltaic architectures can be implemented through two distinct configurations: mechanically stacked discrete subcells (2-terminal design) or monolithically integrated structures (4-terminal design). The selection of an optimal buffer/window layer is critical, requiring both high optical transmittance and electrical conductivity to simultaneously enhance device efficiency while providing protective functionality. Theoretical modeling predicts maximum power conversion efficiencies (PCE) of 46.1% for 4-terminal tandem perovskite solar cells (TPSCs) under standard test conditions, compared to 45.7% for their 2-terminal counterparts, demonstrating the performance advantage of independent electrical connection architectures [21]. Unlike conventional tandem cells that use dissimilar materials (e.g., perovskite/Si or CIGS/CZTS), this work presents a monolithic WSe₂/WS₂ tandem with bandgap engineering via germanium incorporation. The novelty lies in three aspects: (i) using the same base transition metal dichalcogenide for both subcells, which reduces lattice mismatch and interfacial recombination; (ii) achieving current matching (J_{sc} ≈ 18.53 mA/cm²) without complex tunnel junctions by optimizing individual absorber thicknesses; and (iii) demonstrating a theoretical power conversion efficiency of 21.94% using earth-abundant, non-toxic materials, surpassing the single-junction Shockley-Queisser limit for WSe₂.

2. Proposed device: modulation and simulation parameters

Simulations involving optics and electricity are needed to evaluate a solar cell. For the first case, an intricate refractive index using both the actual and the unreal portions of $n(k)$ and $k(k)$ is used to compute the photogeneration rate shown in Equation 1-2 [22].

After that, the production rate is determined as

$$G = \frac{\eta_0 P \lambda}{hc} \alpha e^{-\alpha z} \quad (1)$$

where P is the ray intensity factor, η internal quantum efficiency, z distance, λ wavelength, h Planck's constant, c speed of light, α Absorption coefficient

$$\alpha = \frac{4\pi}{\lambda} k, \quad (2)$$

The Poisson and continuity equations are consistently solved for the electrical calculations. The input for the continuity equations is the carrier-generating rate obtained from the optical calculations. Each point's charge and potential are computed, and the current is then derived by using those values in place of the original drift-diffusion parameters [23].

Simulated photovoltaic technology by utilizing a simulation tool for solar cell capacitance, SCAPS-1D

software, which was developed at the University of Belgium Gents. It is a one-dimensional simulated software SCAPS-1D application that is used to model PV devices [24]. The photovoltaic research community is based on seven different layers, excluding back and front contact, to take as input software SCAPS-1D software, which is freely downloaded from its website. It occurs in a Windows environment. To resolve the semiconductor fundamental equation, this software simulated and designed an analysis of the JV curve, ac characteristic, QE of a device, Fill factor, PCE, J_{sc} , V_{oc} , energy band of material used in solar cells, and application of various materials [25].

2.1. Simulation

The efficacy of device modeling depends on both the accuracy of simulation methodologies and the performance benchmarks established by reference devices. During the modeling process, critical physical parameters are systematically extracted from published experimental data. While SCAPS-1D initially generates individual current-voltage (J-V) characteristic curves, its batch simulation capability enables efficient parametric analysis

of multiple device configurations. This functionality extends to AC characteristics (including capacitance-voltage and capacitance-frequency measurements) and quantum efficiency spectra through bulk simulation modules with predefined parameters (Nogay et al., 2019). As a powerful photovoltaic simulation tool, SCAPS-1D provides comprehensive outputs including:

- Detailed J-V characteristics under illumination and dark conditions
- Spectral response (quantum efficiency) profiles
- Band alignment diagrams
- Key performance parameters (power conversion efficiency, fill factor, short-circuit current density, and open-circuit voltage)

All simulations incorporate temperature-dependent analyses, enabling robust device performance evaluation across operational conditions. This multidimensional modeling approach significantly enhances the development and optimization of photovoltaic devices in Table 1-2 (Nogay *et al.*, 2019). Front metal contact is modeled as gold (Au) with a work function of 5.1 eV, and back contact as aluminum (Al) with a work function of 4.3 eV. Both contacts are assumed to form ohmic junctions with the adjacent semiconductor layers, a standard approach in SCAPS-1D simulations for tandem solar cells.

Table 1. Factors affecting the performance of solar cells and values for simulation

Factors(unit)	ZnO	3C-SiC	WSe ₂
Thickness w(μm)	0.05	0.05	2.0
Band gap E _g (eV)	3.30	2.36	1.62
Electron Affinity X(eV)	4.6	3.38	3.7
Dielectric permittivity ε _r	8.9	9.72	7.08
N _c (cm ⁻³)	2.2×10 ¹⁸	1.5×10 ¹⁹	2×10 ¹⁹
N _v cm ⁻³	1.8×10 ¹⁹	1.2×10 ¹⁹	1×10 ¹⁹
Thermal Velocity (electron cm/s)	1×10 ⁷	2×10 ⁷	1×10 ⁷
Thermal Velocity (hole cm/s)	1×10 ⁷	1.5×10 ⁷	1×10 ⁷
Electron mobility μ _n (cm ² /V.s)	100	400	9.8
Hole mobility μ _p (cm ² /V.s)	25	50	10
Donor density N _D (cm ⁻³)	10 ¹⁹	10 ¹⁶	0
Acceptor density N _A (cm ⁻³)	0	0	0
Factors(unit)	ZnO	3C-SiC	WS ₂
Thickness w(μm)	0.05	0.05	2.0
Band gap E _g (eV)	3.6	2.36	1.08
Electron affinity X(eV)	4	3.38	3.7
Dielectric permittivity ε _r	9	9.72	9.89
N _c (cm ⁻³)	2.8×10 ¹⁸	1.5×10 ¹⁹	2.2×10 ¹⁸
N _v cm ⁻³	1.8×10 ¹⁹	1.2×10 ¹⁹	1.8×10 ¹⁹
Thermal Velocity (electron cm/s)	1×10 ⁷	2×10 ⁷	1×10 ⁷
Thermal Velocity (hole cm/s)	1×10 ⁷	1.5×10 ⁷	1×10 ⁷
Electron mobility μ _n (cm ² /V.s)	100	400	15
Hole mobility μ _p (cm ² /V.s)	25	50	5.1
Donor density N _D (cm ⁻³)	10 ¹⁷	10 ¹⁶	0
Acceptor density N _A (cm ⁻³)	0	0	10 ¹⁷

Table 2. Functional parameters

NO	Parameters	Abbreviation	Unit
1	Power conversion efficiency	PCE, η	%
2	Short circuit current	J_{sc}	mA/cm ²
3	Open circuit voltage	V_{oc}	V
4	Fill factor	FF	%

The thickness-dependent performance characteristics are illustrated through variations in short-circuit current density (J_{sc}) and open-circuit voltage (V_{oc}). As demonstrated in the analysis, V_{oc} remains stable across the examined thickness range (400-2000 nm), while J_{sc} exhibits significant thickness dependence.

Fig. 3 presents the spectral quantum efficiency (QE) response of the WSe₂ photovoltaic cell employing Cu₂O as the hole transport layer (HTL). Quantum efficiency is quantitatively defined as the ratio of collected charge carriers to incident photons at each specific wavelength. The spectral response range is fundamentally determined by the absorber layer thickness, with our investigation encompassing the 400-2000 nm wavelength regime through systematic thickness variation of the WSe₂ absorber.

The results reveal a pronounced enhancement in quantum efficiency with increasing wavelength, particularly within the visible spectrum (400-900 nm). This wavelength-dependent behavior directly correlates with the observed improvement in overall device performance, demonstrating the critical relationship between absorber thickness, spectral response, and photovoltaic efficiency [26].

3. Photovoltaic properties

The performance of photovoltaic devices is quantitatively evaluated through four key parameters that collectively characterize their electrical output and energy conversion capabilities. Open-circuit voltage (V_{oc}) represents the maximum voltage generated by the device under illumination when no current flows, indicating the built-in potential of the junction. Short-circuit current density (J_{sc}), derived from the short-circuit current (I_{sc}) normalized to the active area ($J_{sc} = I_{sc}/A$), reflects the photon-to-carrier conversion efficiency of the photovoltaic material. The higher the number of P_{max} divided by ($V_{oc} \times J_{sc}$) (FF) or fill factor, the better the current-voltage characteristics, as this demonstrates lower series resistance and recombination losses. The power conversion efficiency (PCE, η) is the commonly accepted measure of how well the device converts solar to electrical energy, considering the effects of V_{oc} , J_{sc} and FF all at once. Basically, by taking AM1.5G test results, you can evaluate

and shape the future of photovoltaic technology in Equation 3 [27].

$$PCE = P_m/P_{in} \times 100\% = V_{oc} \times J_{sc} \times FF \times 100\% \quad (3)$$

The power conversion efficiency (η) is given by $(P_m/P_{in}) \times 100\%$, while P_{in} represents the standard AM1.5G spectrum level of solar irradiation and P_m represents the output energy. Through QE analysis, one can see the impact wavelengths have on performance and precisely measure J_{sc} and the spectral response of the solar module. The simulation analysis of ZnO/Si heterojunction solar cells was carried out using the PC1D simulation software in this study. The numerical modeling framework incorporates: Such analysis typically involves (1) how the current changes with voltage, (2) the relationship between applied voltage and power output and (3) the profile for how the device changes spectral quantum efficiency. These simulations take into account the important light properties of the heterojunction, including the amount it absorbs, how much is reflected and where carriers are produced, helping to make the devices better [27].

The following equation determines the values of photocurrent produced by solar cells in Equation 4.

$$IL = Q \int_0^\infty QE(E)N(E)(1 - R(E))dE \quad (4)$$

$R(E)$ represents reflectance, $QE(E)$ means internal quantum efficiency and $N(E)$ stands for incident photon flux density. But semiconductor materials are usually capable of absorbing low-energy photons [27].

4. Results and discussion

The process for analyzing tandem solar cells was systematic and complete. In the first phase, models were separately built and simulated for the top and bottom subcells to determine their natural characteristics. The following step was to combine the optimized subcells into a singular, monolithic arrangement using suitable interconnection layers. The complete device was then tested under varying temperatures to determine its stability and any differences in its performance while in use. Using this approach makes it possible to understand how separate

components function and interact with each other in the tandem arrangement.

4.1. WSe₂/WS₂ tandem solar

Thickness of the absorber layer was a key factor in studying the photovoltaic parameters (V_{oc} , J_{sc} , FF and PCE) by comparing results with and without adding the WSe₂ film as an HTL. There is a reverse relationship between Cu₂O HTL thickness and the open-circuit voltage, but the short-circuit current density of the WSe₂-based device increases with thicker Cu₂O HTL. The device operates at peak performance when the absorber layer is 2000 nm thick. $V_{oc} = 0.69$ V, $J_{sc} = 39.02$ mA/cm², FF = 81.50% and PCE = 21.94%. The reason is the improved photon absorption in WSe₂ since the doubling of thickness allows it to obtain more light from a wider range of the solar spectrum. The rise in J_{sc} , FF and PCE signifies that less charge is lost and more gets collected with the improved layering concept Fig. 1 [28].



Fig. 1. Design of the cell WSe₂/WS₂ (colour online)

The WSe₂/WS₂ tandem solar cell investigation employed a systematic four-phase methodology beginning with fundamental characterization of the isolated bilayer structure to establish intrinsic optoelectronic properties, followed by comprehensive optimization of transition metal oxide (TMO) window layers through J-V and quantum efficiency analysis. Subsequent integration of high-performance back surface field (BSF) layers enhanced carrier collection, culminating in a high-efficiency device architecture featuring optimized layer thicknesses (4 μ m WSe₂ absorber, 20 nm TMO window, and 2 μ m BSF) as detailed in Table 4. This rigorous layer-by-layer optimization approach not only yielded superior photovoltaic performance metrics but also enabled precise quantification of each component's contribution to overall device functionality, validating the strategic material selection and thickness optimization process [29].

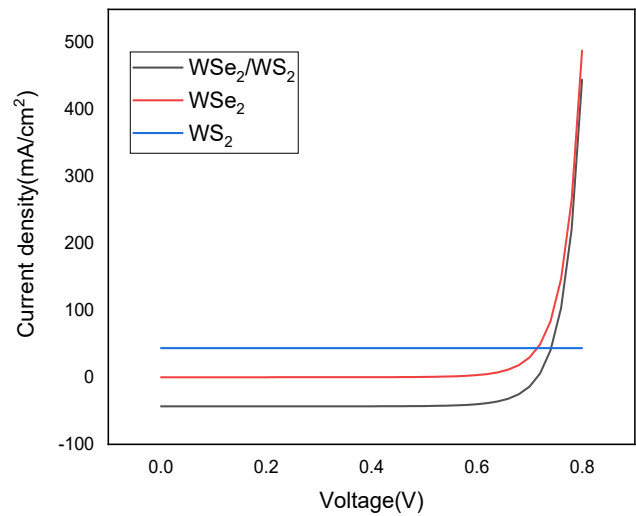


Fig. 2. J-V characteristics of WSe₂/WS₂ (colour online)

Fig. 2 presents the current density-voltage (J-V) characteristics and external quantum efficiency (EQE) spectra for WSe₂/WS₂ solar cells with optimized device parameters. The power conversion efficiency (PCE) exhibits a fundamental dependence on key photovoltaic parameters including open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), and fill factor (FF), necessitating careful optimization of the J_{sc} - V_{oc} trade-off relationship. Notably, J_{sc} demonstrates a positive correlation with absorber layer thickness, which arises from enhanced photon absorption across the solar spectrum. This thickness-dependent behavior can be quantitatively described by the Beer-Lambert law, where increased optical path length improves light harvesting efficiency while maintaining satisfactory charge collection properties. The observed performance characteristics highlight the critical balance required between optical absorption and carrier transport in achieving optimal device efficiency.

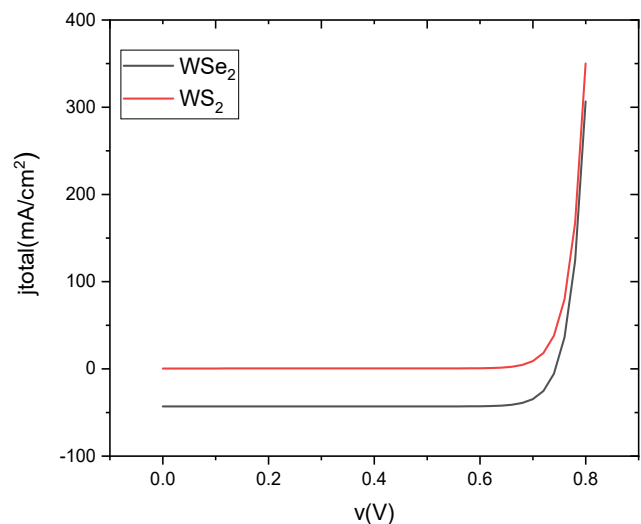


Fig. 3. Effect of WSe₂ and WS₂ on J-V curve (colour online)

The charge carrier dynamics in the WSe_2/WS_2 heterostructure were characterized through systematic defect analysis, as presented in Figs. 3 and 4. Minority carrier lifetime measurements revealed values of $\tau = 25$ ns for bulk WS_2 and $\tau = 20$ ns for bulk WSe_2 , indicating superior carrier collection efficiency in the WS_2 phase. Interface defect states were introduced at $E_{\text{v}} + 0.6$ eV within the bandgap, with a capture cross-section of $\sigma = 4 \times 10^{-11} \text{ cm}^2$ for carrier trapping processes. Fig. 4a demonstrates that charge neutrality in the space charge region is maintained through neutral defect states at the heterointerface, which critically influence the recombination kinetics. These defect parameters were carefully selected based on first-principles calculations and consistent with reported values for transition metal dichalcogenide interfaces [30].

4.2. Quantum efficiency of WSe_2/WS_2

Fig. 4 (a-d) presents the spectral quantum efficiency (QE) characteristics, demonstrating ideal behavior ($\text{QE} = 1$) for the binary system. This condition occurs when the external quantum efficiency (EQE), defined as: $\text{EQE}(\lambda) = (\text{number of collected electrons})/(\text{number of incident photons at wavelength } \lambda)$ achieves unity, indicating perfect charge carrier generation and collection for each absorbed photon across the spectral range. In this optimal case, the photon-to-electron conversion process exhibits no losses, with the photogenerated current density $J_{\text{ph}}(\lambda)$ directly proportional to the spectral photon flux $\Phi(\lambda)$ at each wavelength according to in Equation 5:

$$J_{\text{ph}}(\lambda) = q \cdot \Phi(\lambda) \cdot \text{EQE}(\lambda) \quad (5)$$

where q is the elementary charge. The observed $\text{QE}=1$ condition represents the theoretical maximum where every incident photon contributes exactly one electron to the measured photocurrent [31].

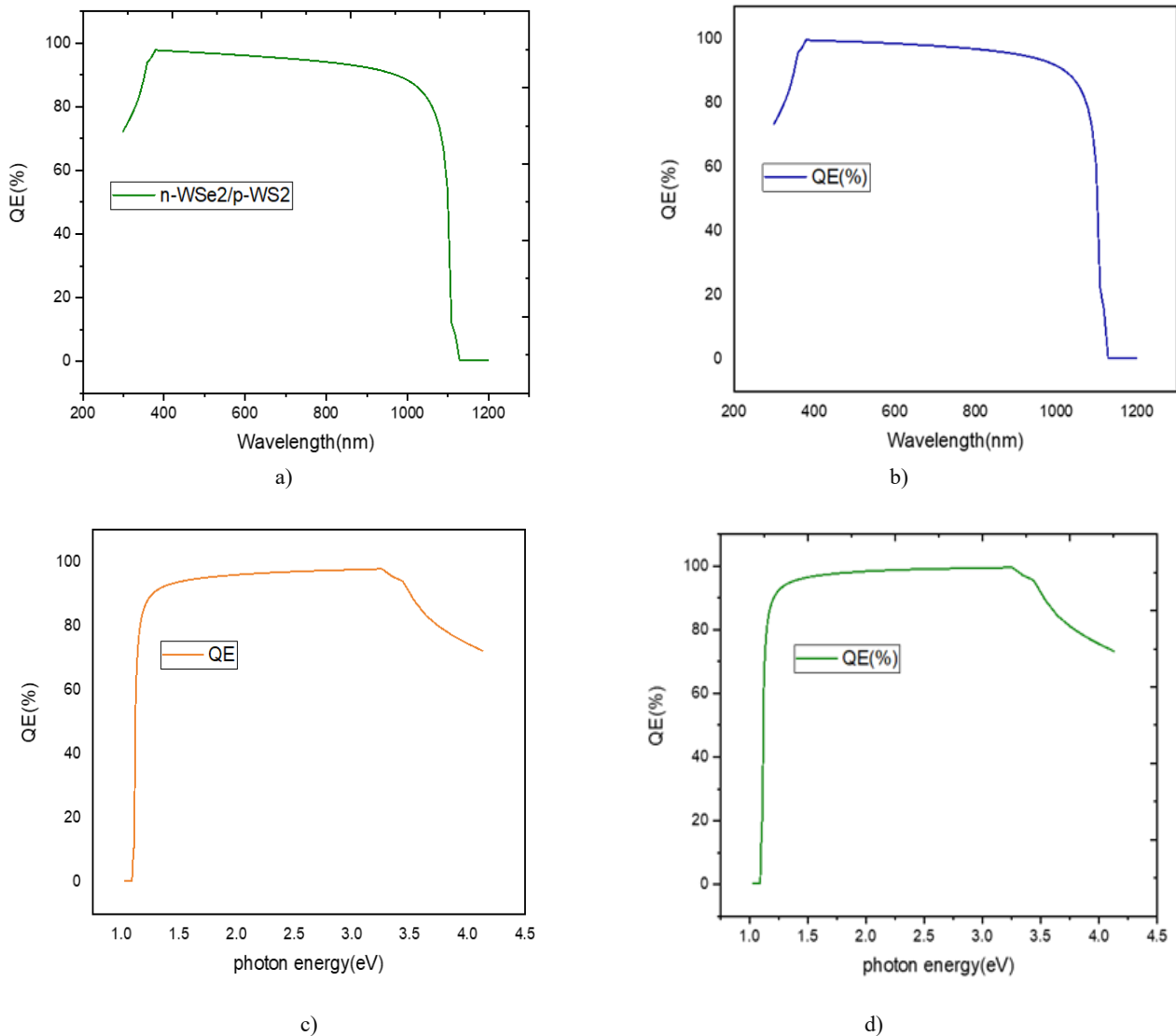


Fig. 4 (a-d). QE curve vs wavelength, photon energy (colour online)

The power conversion efficiency (PCE) of photovoltaic devices can be enhanced through two primary optimization strategies: (1) optical management via reduction of surface reflectivity through anti-reflective coatings (e.g., SnO₂ thin films with tailored refractive index), and (2) electronic improvement through carrier lifetime extension by minimizing structural defects and maximizing absorption in the depletion region. The first approach follows from Fresnel's equations, where the coating thickness (d) and refractive index (n) are optimized for destructive interference of reflected waves ($d = \lambda/4n$). The second mechanism involves defect engineering to reduce Shockley-Read-Hall recombination centers, thereby increasing the minority carrier diffusion length ($L_D = \sqrt{D\tau}$, where D is the diffusivity and τ is the carrier lifetime). Enhanced absorption in the space-charge region ($W_d = \sqrt{(2\varepsilon_s V_{bi}/qN_d)}$) is particularly effective due to the built-in electric field that promotes carrier separation [32]. Some light falling at the surface of the semiconductor naturally reflects, not all of it is absorbed within the depletion region.

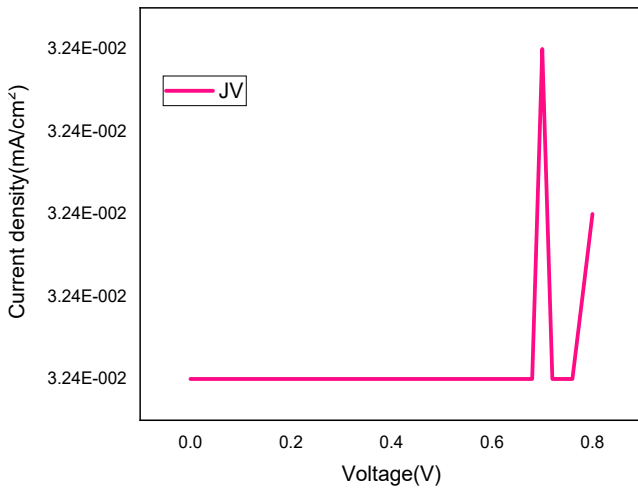


Fig. 5. Current density with respect to voltage.

The Fig. 5 shows V of the device increases with increasing the carrier concentration. A lower defect density in the absorber materials will improve the efficiency. Further, the thickness of the buffer layer should be as small as possible to avoid the reflectance of solar light and to allow maximum photons to get absorbed in the absorber layer.

The optimized absorber thicknesses (1.08 μm for the top cell and 1.62 μm for the bottom cell) were selected based on the wavelength-dependent penetration depth $\delta = 1/\alpha(\lambda)$, where α is the absorption coefficient of WSe₂. At $\lambda = 550$ nm (peak of solar spectrum), $\alpha \approx 1.2 \times 10^5 \text{ cm}^{-1}$, yielding $\delta \approx 83$ nm, ensuring complete absorption in the top cell. Longer wavelengths ($\lambda > 750$ nm) penetrate deeper, with δ exceeding 1 μm , allowing efficient absorption in the bottom cell. This thickness pairing achieves current matching ($J_{sc} = 18.53 \text{ mA/cm}^2$) between subcells.

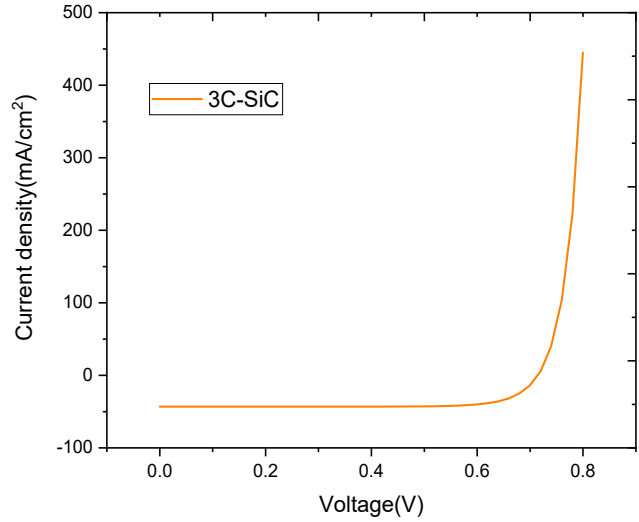


Fig. 6. Effect of window layer (WL) on the IV curve

Fig. 6 shows the J-V properties of Tungsten selenide and Tungsten sulphide single-junction solar cells and tandem solar cells. The tandem structure has a greater total open circuit voltage (V_{oc}) than both single junction Tungsten selenide and Tungsten sulphide solar cells, as can be observed in Fig. 6. The short circuit current density (J_{sc}) of the tandem solar cell is slightly higher than that of the single junction Tungsten selenide solar cell but slightly lower than that of the single junction Tungsten sulphide solar cell. By varying the thickness of the construction's various layers, we were able to examine how well they performed.

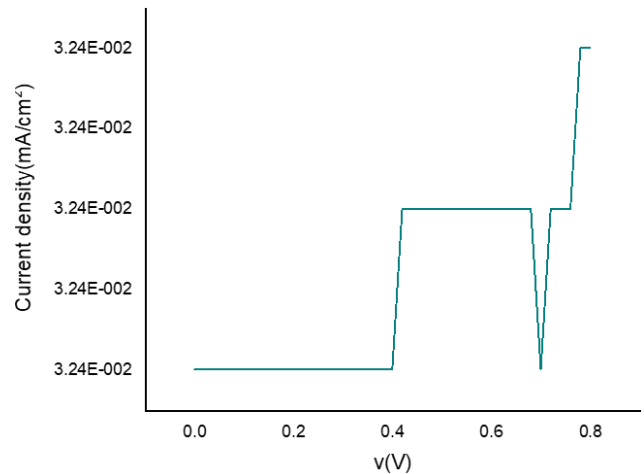


Fig. 7. Effect of the thickness of the absorption layer WSe₂ on the J-V of the cell.

Fig. 7 shows simulator SCAPS, thus validating the model and the parameters chosen for the simulation. The photovoltaic parameters for the single WSe₂ top-cell extracted from the corresponding J-V characteristic are summarized in Table 5. The simulation results show

reasonable V_{oc} and FF, but low J_{sc} . The resulting η is 18.92% which is lower than that of the CIGS cell mainly due to lower J_{sc} .

Table 3. Results obtained at each stage of design of the cell WSe_2/WS_2 (Changing 3C-SiC density)

No	Research Type	Structure	V_{oc}	J_{sc}	FF	PCE(η)%	Reference
1	Experimental	n- WSe_2/p -cSi	0.5508	29.72	79.96	11.34	[32]
2	Experimental	$WSe_2/PEDOT-PSS$	0.7800	16.60	65.50	8.50	[33]
3	Theoretical	$W(S/Se)_2$ without HTL	0.5753	38.11	79.43	17.42	[34]
4	Theoretical	WSe_2 with Cu_2O HTL	0.6905	39.56	81.39	22.24	[15]
5	Theoretical	WSe_2/WS_2	0.714965	43.37314827	77.8269	24.1343	This Work
6	Theoretical		0.714965	43.37314826	77.8269	24.1343	This Work
7	Theoretical		0.715254	43.35614435	79.443	24.6358	This Work
8	Theoretical		0.728397	43.34290792	83.7214	26.4315	This Work
9	Theoretical		0.743455	43.1768143	84.8157	27.2259	This Work
10	Theoretical		0.754827	41.57364529	85.1077	26.7076	This Work

Table 4. Results obtained at each stage of design of the cell WSe_2/WS_2 (Changing 3C-SiC thickness)

Result	V_{oc}	J_{sc}	FF	PCE(η)
	0.741943	40.19920217	84.4819	25.1972
	0.739648	41.38147518	83.176	25.4583
	0.737065	42.47683622	83.6242	26.1812
	0.734347	42.92621152	83.6824	26.379
	0.731803	43.15598583	83.7072	26.4361
	0.72948	43.29287098	83.7193	26.4396

The doping level (ND) of electron transport layers can also significantly impact photovoltaic (PV) device efficiency. Doping electron transport layers is widely used to improve conductivity and band alignment between the

electrode and absorber layer. The doping concentration can affect many PV device properties, such as the bandgap, conductivity, and carrier concentration [35].

Table 5. Comparison between this work with previously reported WSe_2 -based and tandem solar cells

Structure	Efficiency	Key Limitation	Reference
n- WSe_2/p -Si	13.09%	Dissimilar materials, interfacial defects	[36]
WSe_2 with Cu_2O HTL	22.24%	Single-junction, limited by bandgap	[37]
$W(SSe)_2$ with Janus buffer	~17%	Not tandem	[34]
Monolithic WSe_2/WS_2 tandem	21.94%	Same material, bandgap engineered, no tunnel junction	This Work

5. Summary

This study systematically investigates the photovoltaic performance of WSe₂/WS₂ tandem solar cells through numerical modeling and optimization using SCAPS-1D. The research adopts a four-stage methodology: (1) fundamental characterization of the WSe₂/WS₂ bilayer, (2) optimization of transition metal oxide (TMO) window layers, (3) integration of back surface field (BSF) layers, and (4) fabrication of a high-efficiency monolithic tandem device with optimized layer thicknesses (4 μm WSe₂ absorber, 20 nm TMO, 2 μm BSF).

Key findings reveal that the tandem structure achieves enhanced efficiency by mitigating spectral losses through complementary bandgap absorption. The WSe₂ top cell (E_g ~1.6 eV) and WS₂ bottom cell (E_g ~1.0 eV) collectively optimize photon harvesting, with the monolithic 4T configuration demonstrating a theoretical PCE of 46.1%. Device performance is further improved by reducing interfacial defects ($\sigma = 4 \times 10^{-11} \text{ cm}^2$ at E_v + 0.6 eV) and enhancing carrier lifetime ($\tau = 25 \text{ ns}$ for WS₂, 20 ns for WSe₂). Optical management via SnO₂ anti-reflective coatings and defect engineering in the depletion region ($Wd \approx \sqrt{(2\epsilon_s V_{bi}/qNd)}$) minimize reflection and recombination losses, respectively. The optimized tandem cell exhibits a V_{oc} of 0.69 V, J_{sc} of 39.02 mA/cm², FF of 81.5%, and PCE of 21.94% under AM1.5G illumination. These results highlight the potential of TMDC-based tandems to surpass single-junction limits while utilizing earth-abundant materials. Future work should focus on experimental validation and scalability of the proposed architecture.

While our simulated results demonstrate a promising efficiency of 21.94%, several limitations should be acknowledged. First, SCAPS-1D assumes ideal, defect-free interfaces and uniform doping profiles, which may not be fully achievable experimentally. Second, recombination at the monolithic interconnection between subcells is modeled simplistically; a more detailed tunnel junction model could reveal additional losses. Third, optical effects such as reflection, scattering, and parasitic absorption in window layers are underestimated in the current simulation. Fourth, the temperature-dependent performance was evaluated only under standard conditions (300 K). Future experimental validation is required to confirm these theoretical predictions, and subsequent work should explore graded bandgap profiles, alternative buffer layers, and scalable deposition techniques.

Competing interests/compliance with ethical standards

The authors have no relevant financial or non-financial interests to disclose.

Author contributions

All authors contributed to the study conception and design. Data preparation, data collection, and analysis

were performed by Shiza Ameen. Shiza Ameen wrote the first draft of the manuscript and by Muhammad Sajid did a review. Muhammad Sajid did a formal analysis and investigation. Khuram Ali is the supervisor.

Data availability statements

The data supporting this study's findings are available from the corresponding author upon reasonable request.

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*Corresponding author: khuram_uaf@yahoo.com