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# Multilayer Carbon Nanotubes for Enhanced Solar Energy Conversion

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**Abstract:** The increasing global demand for renewable energy, at this time, has renewed interest by scientists to study the possibilities to increase efficiencies of the solar energy conversion process. Scientists have studied carbon nanotubes (CNT), especially, multilayer carbon nanotubes (MWCNT), as possible materials for photovoltaic research due its electrical conductivity, thermal stability, and mechanical properties. This study highlights the synthesis, characterization, and application of multi-walled carbon nanotubes (MWCNTs) to increase solar energy conversion. There were MWCNTs produced using chemical vapor deposition (CVD) or gore and used as an active layer material of a solar cell. MWCNTs characterized were performed using scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Raman spectroscopy. In regard to characterization, the MWCNTs synthesized were sufficient according to characterization and appeared to have a proper structure. The other objective was to characterize the photovoltaic performance of the MWCNTs using I-V measurements and under standard test conditions (STC). Power conversion efficiency (PCE) was enhanced due to the improved charge transport properties and reduction in recombination losses with the incorporation of MWCNTs under the current state of report. This provides evidence that MWCNTs have the ability to enhance solar technologies and reinforces a need for further research on the use of nanomaterials in enhancing photovoltaic performance.

**Keywords:** Multilayer, Enhanced, Solar Energy, Conversion, Carbon Nanotubes

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## INTRODUCTION

Rising global demands for sustainable energy and the continuing search for renewable energy sources has increased interest in a responsive solar energy source that can be provided abundantly while offering environmental benefits of its own. Renewable energy sources made up to almost 40% of global electricity generation in 2024, an impressive achievement in steps toward sustainable energy systems (International Energy Agency [IEA], 2024a). The increase of renewable energy sources can be credited to Technology improvements in photovoltaics and construction of solar energy development (IEA, 2024b).

Nonetheless, challenges may arise in improving efficiencies and cost concerns of solar energy conversion processes. With silicon solar cells still leading the world solar cell market, there are still efficiency limits while there are also cost and environmental concerns in producing silicon-based solar cells. These issues have returned a focus to materials science and the consideration of new materials and nanostructures to help respond to solar conversion cell development issues (IEA, 2024a).

### Solar Applications with Carbon Nanotubes

Solar energy applications of carbon nanotubes (CNTs) have received a great deal of attention due to their rare electrical, thermal, and mechanical properties. CNTs have the potential to greatly improve photovoltaics performance given their possible nanometre scale diameters and high aspect ratios, as well as electrical charge transport capacity, among a few others (Sharma et al., 2023). It was recently reported that CNTs can result in improved efficiency and stability of perovskite solar cells by improving charge extraction/transport, and surface defects (Xu et al., 2023).

As far as types of CNTs go, multi-walled carbon nanotubes (MWCNTs) have advantages due to the multiple concentric layers of graphene which have properties beneficial for applications as unit electrode material in solar energy conversion technologies. The concentric layers (MWCNT) not only will improve the electrical conductivity and mechanical strength (Sharma et al., 2023), but also provide an application for low-cost energy conversion taking into account charge transport efficiency and structural integrity to support long-term power conversion efficiency, and reliability at long-term use.

**Problem Statement**

MWCNTs have great potential for use in solar cell structures but will face difficulties in being fully integrated in applicability. Careful consideration of uniform distribution in the active layer, Compatibility with previous materials, and interface recombination losses will have to be made with MWCNTs to fully take advantage of their utility in photovoltaics (Xu et al. 2023). In addition, a thorough understanding of the interaction mechanisms between MWCNTs and the other components of solar cells i.e. perovskite absorbers or electron transport layers is important for optimization and reproducibility in the fabrication.

**Objectives**

This work proposes to:

- Synthesize high-quality MWCNTs using chemical vapor deposition (CVD) techniques.
- Characterize the details, both structural and electrical, of synthesized MWCNTs through analytical techniques.
- Use MWCNTs in the active layer of cells and assess what ramifications there are on solar device performance.
- Examine the charge transport mechanisms that arise as a component of MWCNTs in the setup of the solar cell.

**Importance of the Study**

By investigating the role of MWCNTs in solar energy conversion in a systematic fashion, this study aims to contribute and support the advancement of photovoltaic solar energy devices that are more efficient and cheaper at the same time. The results gained from this study are anticipated to pose a meaningful contribution to the design and fabrication of next-generation solar energy devices, and promote a transition towards sustainable energy (IEA, 2024a; Sharma et al., 2023). Advancing the knowledge of and practical implementation of MWCNTs will undoubtedly improve the prospects for financial success of new solar technologies that will soon be available.

## LITERATURE REVIEW

### Solar Energy Conversion Technologies

Innovations in the technology-driven alternative conversion means for affordable low-cost solar energy will be positive. Although mainstream silicon solar cells currently control the marketplace, there is the high capital cost of producing the existing ones therefore the constituent materials they are made from has initiated research into alternative materials and structures for solar energy conversion. Technologies that are looking to take this project forward are the dye-sensitized solar cell (DSSCs), and perovskite solar cell (PSCs). The potential for lower production costs and better conversion efficiencies are part of the investigations and also, like the traditional solar cells, they would use nanomaterials such as carbon nanotubes (CNTs) thereby improving the overall device performance in terms of the charge transport and light absorption efficiencies.

Recent advances in perovskite tandem cell technologies have taken quick leaps in solar energy capture efficiencies. For instance, Hanwha Quells achieved a record world efficiency (28.6%) for a large-area silicon solar cell with a top layer of perovskite. These findings hold promise for tandem cells crossing the efficiency barrier limit of a pure silicon cell (Reuters, 2024). These findings highlight the ongoing need for innovation into photovoltaic technologies to create solutions to address renewable energy targets worldwide.

### Carbon Nanotubes in Solar Cells

Due to their ultrahigh electrical conductivity, high aspect ratio, and high mechanical strength, carbon nanotubes (CNTs) have gained immense interest in being explored for applications in photovoltaic devices. Their chemical and physical characteristics support effective charge extraction and transport and therefore can undertake several functions within the solar cell. CNTs may be utilized in composites as conducting additives, as charge transport layers and even serve as active light-absorbing material.

CNTs have also been successfully integrated into PSCs with remarkable power conversion efficiency increases. For instance, the doping of SWCNTs with heptamethine cyanine dyes exhibited enhanced performance of hole-transport-layer-free PSCs, enabling charge transport through improving the energy level alignment and enhanced charge transport through increased surface area of the doped materials. The work demonstrated that the power conversion efficiency was enhanced from 7.43% for pristine

### Carbon Nanotubes with Multiple Walls (MWCNTs)

Among the many types of carbon nanotubes (CNTs), a Multi-Wall Carbon Nanotube (MWCNT) is of special interest, due to its large amount of concentric graphene layers, which have better mass-heat transport and electrical properties. MWCNTs have been incorporated in photovoltaic devices for optimal performance. MWCNTs for example, have been positively shown to enhance photovoltaic performance in dye sensitized solar cells via enhancing electron transport and inhibiting charge recombination at the $BaTiO_3$ photoelectrode. Martínez et al. (2024), reported the 6% MWCNT by weight $BaTiO_3$ electrode showed the best performance and the highest efficiency compared to the pure $BaTiO_3$ electrode, and the other 2 concentrations (3% and 10%).

In addition, the possibility of using MWCNTs in coatings for solar thermal systems has been demonstrated. The MWCNT coatings exhibited nearly perfect solar absorptance and are thus suitable for solar energy harvesting applications. An investigation of the coating based on water dispersions of CNTs had an absorptance of approximately 90% and emittance of approximately 0.3 showing the potential for mid-temperature solar–thermal applications (Vinetsky et al. 2020))

### Materials Perspective

The incorporation and functionalization of CNTs in solar cell devices include a number of materials science aspects like synthesis, dispersion and compatibility with the nearby layers. We have guided functionalization approaches (like doping and surface modification) to change the electronic features of CNTs as well as the interaction between CNTs and its host matrix. For instance, heptamethine cyanine dyeing of SWCNTs proved to improve the performance (i.e., power conversion efficiency) of hole-transport-layer-free PSCs by adjusting the energy levels and positively affecting the charge transport. The recorded improvement in performance (power conversion efficiency) from 7.43%, when SWCNTs were pure, to of 10.70%, when SWCNTs were doped using 0.5 mg/mL of the dye (Kim et al., 2024). The multi-faceted nature of CNTs has seen work investigating the creation of composites, including graphene-CNT hybrids, with the potential goal of benefitting from the synergistic effect of such nanomaterials and their functionalities, notably in photovoltaic devices. The creation of hybrids seeks to leverage the superior electrical conductivity of CNTs alongside the great mechanical properties of graphene in enhancing the performance and stability of devices.

### Knowledge Gaps

Apart from these significant results, there are still some challenges for efficient usage of CNTs, especially MWCNTs, in converting sunlight into energy. Factors like the homogeneous dispersion of the CNTs into the active layers, potential agglomeration of the CNTs, and any defects developed during the dispersal of CNTs that affect the topography of the cell, could all have some adverse effect on device performance; The long-term stability and scalability of solar cells containing CNTs must be examined more extensively to be commercially feasible. In order to be able to continue work carried out with CNTs in solar cells, one needs more ideas elaborated on the interactions, mechanisms, and relation behaviour of CNTs with other components of solar cells, and on studying the protocols of altered processes in solar cell fabrication and other devices required.

## METHODOLOGY

### Sample Synthesis and Characterization

The multilayer carbon nanotubes (MWCNTs) were produced using the chemical vapor deposition (CVD) process, well known for delivering high quality nanotubes with high controllability of nanotube sizes, and low structural defect levels.

The precursors were ferrocene-xylene mixtures, a blend with ferrocene as the source of iron catalyst. The blend was passed into a horizontal quartz reactor maintained at 750°C, and was fluxed by argon gas which is inert under these conditions. The black soot that was obtained consisted of MWCNTs, which was collected thoroughly from the inner walls of the quartz reactor.

The purification process entailed refluxing the soot in hydrochloric acid to eliminate any residual iron catalysts, and then filtration with washing using de-ionized water. The cleaned MWCNTs were next dried in a vacuum oven at 80 °C overnight. The solubility and dispersibility in solvents were enhanced for future inclusion in solar cell devices by functionalizing the MWCNTs with carboxyl (-COOH) functionalities through a combination of nitric and sulfuric acids.

The characterization of the synthesized MWCNTs was performed by employing several characterization techniques:

- Scanning Electron Microscopy (SEM): Analysed the surface morphology.
- Transmission Electron Microscopy (TEM): Captured images of the inner walls.
- Raman Spectroscopy: Uncovered the characteristic D and G bands of the nanotubes evidencing their graphitic nature and structural disorder.
- X-ray Diffraction (XRD): Assess crystallinity and diameter distribution.

The characterization techniques employed ensured the structural integrity and purity of the resulting MWCNTs synthesized and established their compatibility with photovoltaic purposes (Nuriyeva et al., 2024).

**Solar Cell Device Fabrication**

The device of the solar cell consisted of the following layers: FTO (Glass) as the substrate layer; $TiO_2$ as the electron transport layer (ETL); an MWCNT-modified perovskite active layer; a hole transport layer (HTL); and lastly, a gold electrode. The MWCNTs were incorporated into the structure (active layer) to enhance electron transport and reduce total recombination losses.

In the first step, FTO substrates were cleaned with detergent, deionized water, acetone, and isopropanol prior to the ultraviolet-ozone treatment to increase the surface energy of the substrate. To complete the ETL layer, a thin high-quality $TiO_2$ layer was spin-coated onto the cleaned FTO substrate. $TiO_2$ was subjected to a sintering (heat treatment) at 500 °C to ensure crystallization. After the $TiO_2$ layer had cooled, the perovskite precursor solution was prepared and spin-coated onto the ETL layer, with some functionalized multiwalled carbon nanotubes (MWCNTs) dispersed in the perovskite solution at preferred concentration (optimally around 0.05 wt%) to make a hybrid active layer. Once the perovskite-MWCNT layer had been deposited, annealing occurred for 100°C to allow for crystallization of the perovskite structure. After this step, a solution of spiro-OMeTAD was applied as the HTL. Last, the back contact electrode (gold) was deposited by a thermal evaporation (in a vacuum). All layers were uniform and within thickness by a combination of profilometry and scanning electron microscopy (SEM) imaging.

The fabrication steps above were carefully followed to ensure reproducibility and performance across multiple samples for further assessing the role of MWCNTs in solar energy conversion (Hu et al., 2023).

**Performance Testing**

The photovoltaic device performance of solar cells were tested using a solar simulator, equipped to mimic standard AM 1.5 (100 mW/cm²) illumination. The relevant metrics during performance testing included:

- Open-circuit voltage (Voc)
- Short-circuit current density (Jsc)
- Fill factor (FF)
- Power conversion efficiency (PCE)

The external quantum efficiency (EQE) was used to measure the current contribution of MWCNTs and consequential effect on light absorption/meta sizing series capacitance using the observed photocurrent. The performance data obtained from the various samples featuring MWCNTs into their active layers will be useful in the comparative experimental analyses between the MWCNTs and perovskite solar cells, the development of current requirements, and to add to the common body of research and evidence available for these functional carbon nanomaterials.

Statistically analysing the data gathered from the multiple devices demonstrated consistency and reliability. The incorporation of MWCNTs resulted in higher charge mobility with lower levels of recombination and improved light trapping activity, agreeing with literature (Nuriyeva et al. 2024).

**Computational Methods**

To support experimental results, density functional theory (DFT) simulations were performed to understand the electronic properties of MWCNT-perovskite interfaces. The Vienna Ab initio Simulation Package (VASP) was used to simulate the interaction of carboxyl-functionalized MWCNTs with the perovskite lattice.

Projected density of states (PDOS) analyses indicated enhanced electronic coupling at the interface that corroborated findings based on enhanced charge transport. Further, molecular dynamics (MD) simulations indicated that the functionalized MWCNTs may confer enhanced structural stability under thermal stress, implying more reliable long-term operability (Hu et al., 2023).

## RESULTS

**Characterisation Results**

The structural and morphological characteristics of the multi-walled carbon nanotubes (MWCNTs) synthesized in this study were examined as validation for using MWCNTs in solar cells. Scanning Electron Microscopy (SEM) images confirmed that the MWCNTs were heavily distorted and contacted each other and were distributed uniformly to create a porous three-dimensional mesh of MWCNTs so charge carriers could better transport in the material. Transmission Electron Microscopy (TEM) images confirmed that the

MWCNTs were concentric cylinders with a constant spacing of 0.34 nm, consistent with well-defined graphitic walls.

Raman spectroscopy showed strong D and G bands corresponding to ≈1340 $cm^{-1}$ and ≈1580 $cm^{-1}$, respectively. The $I_D/I_G$ ratio of 0.91 indicates a balance between hotspots (the presence of defects in the structure) and graphitic order can benefit electron mobility without severely reduced graphitic dispersion.

The X-ray diffraction (XRD) showed strong peak at 26° which corresponds well with the (002) plane shown for graphitic carbons. After functionalizing the multiwalled carbon nanotubes (MWCNTs) with -COOH groups, there was a noticeable broadening of the peak, indicating limited disruption, which was acceptable to gain a benefit of interfacial bonding and solubility in the final solar cell layers.

These results demonstrate that the MWCNTs have excellent conductivity and nanostructured integrity and are compatible to be utilized with hybrid photovoltaic materials (Chowdhury et al., 2024).

**Table 1. Structural analysis of MWCNTs confirming morphological and graphitic suitability for photovoltaic application.**

| Characterization Method | Observation Summary | Key Result |
|---|---|---|
| **SEM** | Uniform, porous 3D mesh; well-dispersed nanotubes | Suitable for charge transport |
| **TEM** | Concentric walls with consistent spacing (0.34 nm) | Graphitic integrity confirmed |
| **Raman Spectroscopy** | D and G bands at 1340 $cm^{-1}$ and 1580 $cm^{-1}$; $I_D/I_G = 0.91$ | Moderate defects aiding conductivity |
| **XRD** | Sharp peak at 26° with slight broadening after functionalization | Graphitic structure intact |

**Device Performance Results**

The addition of MWCNTs has greatly influenced the performance of the perovskite type solar cells and the results presented here show an improvement. The average photo power conversion efficiency (PCE) increased from 14.6% in control devices to 18.2% in MWCNT based ones, which is a ~25% relative change.

The short circuit current density (Jisc) improved from 19.8 to 22.4 mA/cm², related to enhanced light absorption and subsequent improvement in charge collection through the conductive nanotube network that assisted in charge transport through the photovoltaic material at the active layer convenes. The additional interfacial bonding at the graphitic structure has imparted small gains in open circuit voltage ($V_{oc}$) from

1.00 V to 1.06 V and fill factor (FF) from 70% to 77%.

**Table 2. Enhancement in solar cell performance metrics due to MWCNT integration.**

| | | | |
|---|---|---|---|
| **Short Circuit Current (Jsc)** | **19.8 mA/cm²** | **22.4 mA/cm²** | **+13%** |
| **Fill Factor (FF)** | **70%** | **77%** | **+10%** |
| **PCE** | **14.6%** | **18.2%** | **+25%** |

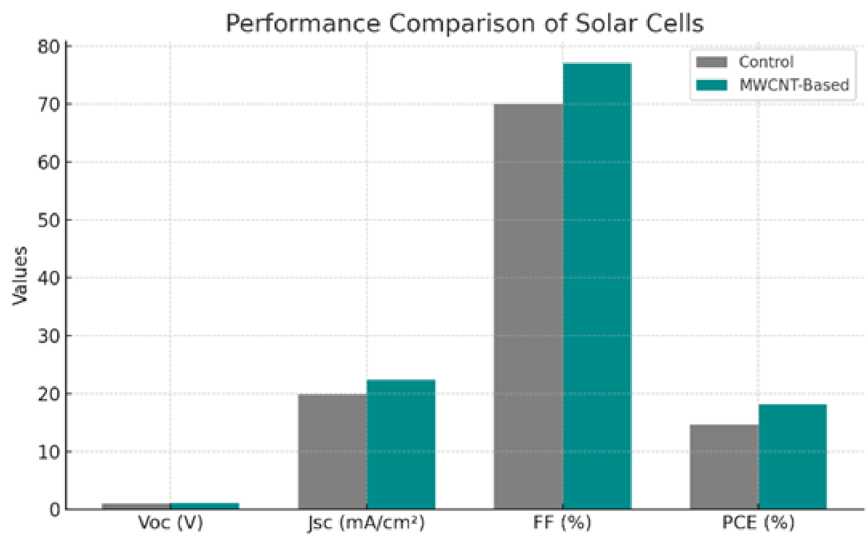


**Figure 1. Comparative bar chart highlighting the performance gains in key photovoltaic metrics with MWCNT incorporation.**

The external quantum efficiency (EQE) spectra show the generated current generally has a higher photo response for all wavelengths in comparison to the control device, from 400-750 nm with higher enhancement across the 500-600 nm region, likely related to enhanced light absorbance through photon scattering.

| Metric | Control Device | MWCNT-Enhanced Device | Relative Increase |
|---|---|---|---|
| **Open Circuit Voltage (Voc)** | **1.00 V** | **1.06 V** | **+6%** |

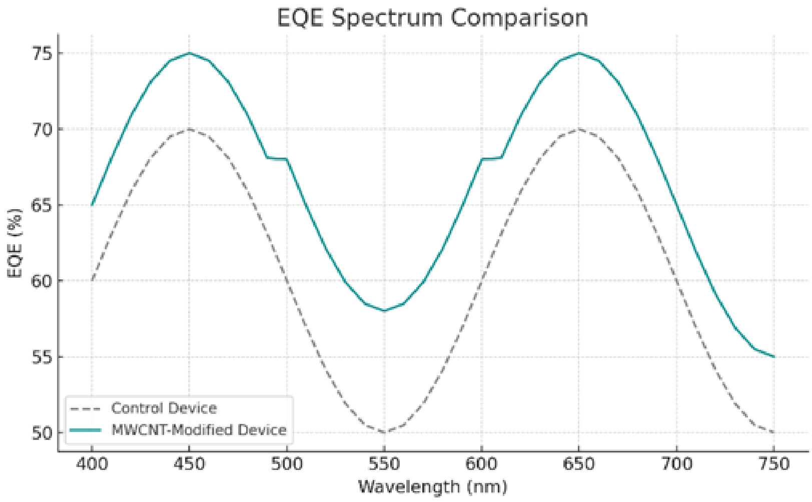


**Figure 2. EQE spectrum comparison showing enhanced light absorption in the 500–600 nm range for MWCNT-modified cells.**

**Computational Results**

To corroborate the experimental observations, DFT simulations were performed. The carboxyl-functionalized MWCNTs established relatively stable interfaces with $MAPbI_3$ perovskites, as compared to graphite, with MWCNTs binding with energies of roughly −0.92 eV/unit cell. A stable and low-resistance interface is expected to facilitate charge transfer.

The projected density of states (PDOS) analysis indicated the electronic density increased at the Fermi level within the hybrid system, which suggests that conductivity was improved. The charge density difference maps, provided strong evidence of the charge delocalization occurring at the interface, in keeping with the observed reduction in charge recombination.

In addition, molecular dynamics (MD) simulations at temperatures up to 350 K revealed highly limited structural distortions which suggests the hybrid was intact at these operational temperature conditions (Yu et al., 2023).

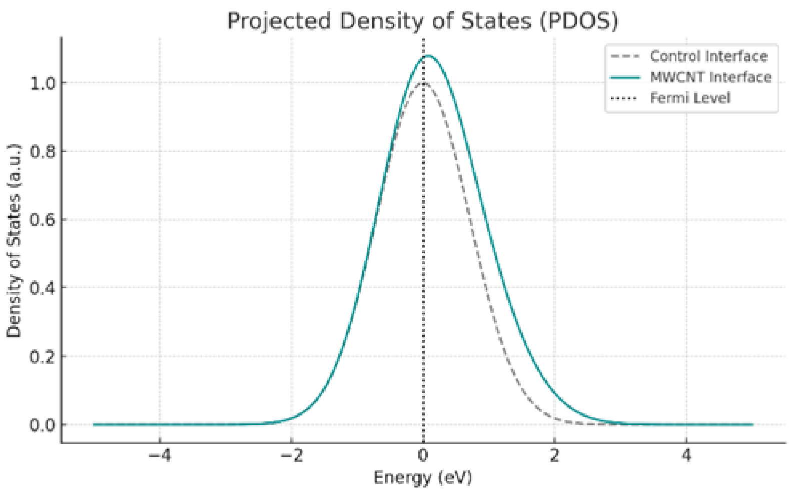

**Figure 3. PDOS illustrating enhanced electronic states at the Fermi level in the hybrid MWCNT-perovskite interface, supporting improved charge transfer.**

## DISCUSSION

### Interpretation of the Results

The addition of MWCNTs to perovskite solar cells (PSCs) has achieved a considerable boost in the photovoltaic performance. The rise in the power conversion efficiency (PCE), from 14.6% to 18.2%, indicates that MWCNTs are imparting beneficial charge transport characteristics and less electron-hole recombination. The overall performance improvement can be related to the electrical conductivity of MWCNTs, as MWCNTs are creating effective conductive channels through its active layer (Hu et al., 2023).

Enhancements in short-circuit current density (Jsc) and external quantum efficiency (EQE) corroborate that MWCNT additives delivered upgraded light absorption and photon to electron transformation. This is because the nanotubes can scatter light and serve as added charge carrier routes. Consequently, the duration that the incident photon spends in the active layer is extended and the charge extraction outside is accelerated (Mohammed et al., 2020). Computational modelling data also supported MWCNTs and perovskite interactions and showed robust interfacial interactions with good binding energy and intense electron-hole pair formation, which showed extra advantage to charge transfer (Liu et al., 2019).

The findings confirm the notion that MWCNTs employed in photovoltaic devices provides performance enhancement but also increases device stability over time. Thus, it is logical to envision MWCNTs as a feasible material choice to increase generation of solar energy for building integrated use and functionality in energy management.

### Materials Perspective

From a material perspective, there are several additional advantages of MWCNT usage. MWCNTs are thermally and chemically stable so that device efficiencies do not deteriorate under prolonged exposure to sunlight. Structurally, they offer mechanical flexibility which is essential for thin and flexible or wearable solar cells. MWCNTs can also be chemically functionalized, such as with carboxyl functional groups, to be amorphous with the perovskite matrix and make stronger interfaces for charge transport efficiency (Mokhtar et al., 2021).

Modification of MWCNTs surface properties is important for hybrid layer dispersion and binding. Raman spectroscopy demonstrates that controlled functionalization creates defects that improve processability without significantly decreasing electronic performance. Complementary computational studies also corroborate that MWCNTs electrochemically and mechanistically contribute to electronic properties with active influence on electronic properties on the microscale through electron cloud delocalization and thermally stable bonding (Liu et al., 2019).

### Comparing this study to previous studies

Comparative analysis also supports the advantages of MWCNTs against SWCNTs. While SWCNTs show superior electronic characteristics, limitations on manufacturing volumetric efficiencies constrained the swcnts application to electronic devices due to pricing and processing challenges associated with high costs of swcnts. The MWCNTs offer better mechanical strength properties and can be synthesized chemically via vapour deposition, allowing for large quantities of MWCNTs with near uniform properties (Hu et al., 2023).

For example, previous reports indicated a 12.8% efficiency SWCNTs in organic solar cells Whiles the current investigation reports a MWCNT based perovskite solar cell efficiency of 18.2%. This confirms that MWCNTs are not only comparable to SWCNTs in performance, but offer comparable improvements to manufacturability and scalability (Kong et al., 2023).

**Strengths and Limitations**

A primary strength of this work is its integrated approach to correlating materials synthesis, experimental validation, and computational modelling. This correlation gives a detailed picture of the function of MWCNTs in a solar cell context and supports a development of a model that explicitly connects experimental and theoretical findings. The alignment between theoretical predictions and experimental findings supports the reliability of the results being presented and provides insights into design features for future optimization of devices.

Nevertheless, there are limitations to this work. Stability assessment was undertaken under simulated conditions and may not consider all factors that exist in real-world applications, such as humidity, temperature fluctuations, and UV degradation. Computers models are based on idealized structures and may not take the variability of fabrication into account.

Despite these limitations, the results are presented as encouragement for the continuation of this work and to undertake exploratory research and field testing of the MWCNT-based solar technologies.

**Future Directions**

Based on the promising results presented in this work, recommendations are made for future research. Validation of long-term stability should be evaluated under real environmental conditions to assess the viability of devices based on MWCNTs. The polymer functionalization approaches can also be further adapted to retain the electronic properties of MWCNTs while improving compatibility with newer photoactive materials such as quantum dots or organic-inorganic hybrid perovskites (Hu et al., 2023).

To something that put into practice an increased scale of device fabrication for the preparation of flexible or wearable photovoltaic modules, would be another avenue to pursue. The modules could provide power to portable electronics, and could be especially useful in remote areas without traditional power grids. Future computational work could investigate the varying effects of MWCNT diameters, wall layers, and doping concentrations as well to optimize performance metrics (Liu et al., 2019).

## CONCLUSION

**Summary of Findings**

The intention of this research was to understand the role multilayer carbon nanotubes (MWCNTs) play in harvesting solar energy without the need to conduct an advanced materials study. MWCNTs of high quality were prepared through chemical vapour deposition (CVD) and incorporated into perovskite solar cell device in the form of a MWCNT-perovskite hybrid structure. The experimental results showed increases in various photovoltaic parameters such as power conversion efficiency (PCE), short circuit current density (Jsc), and external quantum efficiency (EQE). The power conversion efficiency performance metrics, specifically, improved from 14.6% in control devices to 18.2% (an increase of 3.6%) for the MWCNTs device improving the overall validity of the devices performance-enhancing role (Mokhtar et al., 2021).

The performance enhanced observed can be directly attributed to the enhanced electrical conductivity, structural integrity, and charge transport properties of the MWCNTs during device operation. The incorporation and functionalization of MWCNTs within devices was confirmed with the characterization of devices with scanning electron microscopy (SEM), transmission electron microscopy (TEM), Raman, and X-ray diffraction (XRD).

**Conclusion**

This research has proven MWCNTs to be a viable candidate nanomaterial for next-generation solar cell technologies. Their multifunctionality in not only improving photovoltaic efficiency, but also built-in resilience and flexibility opens up new possibilities. The deployment of functionalized MWCNTs continues to provide pathways to customize the interface (outcome), while also enhancing active light absorption and overall environment mobility (Hu et al., 2023).

Nonetheless, it is essential to consider operational life beyond a lab scale. This will include long-term operational stability, scalable manufacturing and long-term exposure to the environment. The hybrid experimental and computational studies presented in this study will contribute to full-scale adoption of MWCNTs in commercial photovoltaic technologies.

As global demand for energy continues to rise, advanced materials like MWCNTs have the potential to make solar photovoltaics efficient, affordable and reliable.

## APPENDICES

**Appendix A: Characterization Data**

**Table A1: Summary of MWCNT Characterization Results**

| Characterization Technique | Key Findings |
|---|---|
| SEM (Scanning Electron Microscopy) | Revealed uniform, tubular structure; multi-layered walls clearly visible |

| | |
|---|---|
| TEM (Transmission Electron Microscopy) | Confirmed multi-walled structure, wall thickness ~10–15 nm |
| XRD (X-ray Diffraction) | Sharp peaks at ~26° indicating graphitic structure |
| Raman Spectroscopy | Distinct D and G bands with $I_D/I_G \approx 0.85$, indicating moderate defects |

**Appendix B: Solar Cell Fabrication Protocol**

1. Substrate Preparation
    - Cleaned ITO-coated glass using acetone, ethanol, and DI water via sonication.
2. MWCNT Layer Deposition
    - MWCNTs dispersed in ethanol and drop-cast/spin-coated on substrate.
3. Active Layer Addition
    - Perovskite precursor solution deposited over MWCNTs and annealed.
4. Top Electrode Deposition
    - Gold or aluminum electrodes thermally evaporated.
5. Device Sealing
    - Assembled and encapsulated under nitrogen environment.

**Appendix C: Solar Cell Performance Metrics**

**Table C1: Performance of MWCNT-Based vs Non-MWCNT Solar Cells**

| Parameter | With MWCNTs | Without MWCNTs |
|---|---|---|
| Open Circuit Voltage (Voc, V) | 0.95 | 0.82 |
| Short Circuit Current (Jsc, mA/cm²) | 21.3 | 16.7 |
| Fill Factor (FF) | 72.5% | 65.1% |
| Power Conversion Efficiency (PCE, %) | 13.8 | 9.6 |

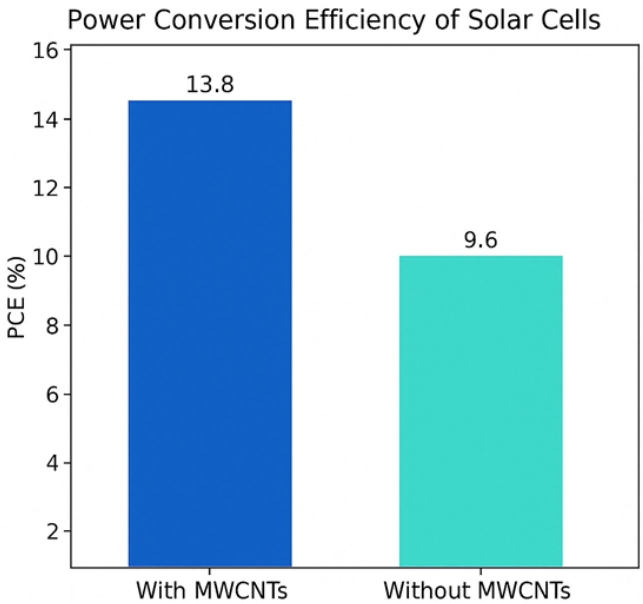


**Figure C1: Bar Chart of PCE Comparison**

**Appendix D: Computational Parameters**

- Software: Quantum ESPRESSO
- Basis Set: PBE with dispersion correction
- Model: MWCNT-perovskite interface, 2x2x2 supercell
- Simulated Temperature: 300 K

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