LAIDLAW SCHOLARS RESEARCH AND LEADERSHIP PROGRAMME 2025 - 2026

INVESTIGATING THE IMPLEMENTATION OF NANOMATERIALS IN PEROVSKITE SOLAR CELLS (PSC) AND THEIR ABILITY TO ENHANCE THE CELL'S STABILITY, EFFICIENCY, DURABILITY, AND LARGE-SCALE APPLICATION

SUMMER 1 RESEARCH REFLECTIVE REPORT

BEATRICE WHARTON-HOOD

SUPERVISOR: DR AMIR PAKDEL

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1. Introduction

As the world continues to reduce its reliance on fossil fuel-generated electricity, the role of renewable and efficient energy systems will grow in magnitude and importance. In particular, industries such as solar energy and photovoltaics (PVs) play a vital role in ensuring the global energy demand is met whilst adhering to environmental regulatory standards. "By 2029, solar energy is predicted to be the biggest generator of renewable energy, and by 2030, the industry is expected to produce 8 225 TWh of energy globally (International Energy Agency, 2024)." Hence, developing solar PVs that can maximise efficiency and have a sustainable life cycle from creation to afterlife is crucial for ensuring the industry's success.

While 1st and 2nd generation PVs such as mono and polycrystalline silicon-based panels have proven to effectively convert solar radiation into electricity, emerging 3rd generation technology such as Dye-sensitised Cells and Perovskite Solar Cells (PSCs) have been able to improve and expand upon the advances made by the industry. PSCs are a form of solar PVs that utilise the perovskite compound material as its active layer. This material, which is arranged in an ABX_3 structure (Suresh Kumar and Chandra Babu Naidu, 2021), is typically found in the form of methylammonium lead iodide $(CH_3NH_3PbI_3)$ and formamidinium lead iodide $(CH(NH_2)PbI_3)$ (Zuo *et al.*, 2016). This active layer of perovskite is just 1 of the 6 layers within the cell itself, with its main purpose being to absorb the photons from solar radiation and to transfer them to the charge transport layers (Zhou *et al.*, 2018).

These 3rd generation cells have improved power conversion efficiency (PCE), with some laboratory-curated PSCs generating 25% PCE under controlled conditions (Kim *et al.*, 2020). In addition, these cells have also shown to utilise low-cost manufacturing methods and readily available materials (Danielyan *et al.*, 2025). However, disadvantages such as the occurrence of lead leakage, restricted durability and stability, and reduced efficiency after large-scale manufacturing have limited the expansion of PSCs. Without addressing these key issues, the potential of PSCs will never be fully realised.

One developing solution to these concerns is using nanomaterials as additives within the active layer of PSCs (Zuo *et al.*, 2016). While there are already examples of nanomaterials being incorporated into layers such as the electron and hole transport layers (Mohammed, 2024; Wu *et al.*, 2025), researchers are investigating whether these materials, when incorporated into the active layer, can extend the lifetime of PSCs while reducing instances of lead leakage and maximising key performance characteristics such as PCE.

2. Methodology and structure of research

This research project was split into 3 key deliverables. The first was to conduct a literature review on PSCs, specifically on the perovskite compound and its nature, the structure and function of each layer in the cell, methods used for to manufacture the cell, and advantages and disadvantages. This was to establish a background understanding of how PSCs function, as well as identifying and communicating key issues hindering its evolution. The second deliverable was to conduct another literature review on the history of nanomaterials in PSCs and their utilisation within the various layers of the cell. This review allowed for the identification of nanomaterials that have already been used experimentally in PSCs, specifically in the active layer. These materials included carbon nanomaterials such as carbon nanotubes, graphene, and carbon quantum dots, MXene-based nanomaterials and Titanium Oxide. These materials were selected based on the magnitude of available literature. Once these materials were identified, a further analysis on their key electronic, electrical, chemical, and mechanical properties was completed.

Once a base understanding was created on both nanomaterials and PSCs, the third deliverable was to investigate if and how the inclusion of the specified nanomaterials improved the efficiency, stability and durability, manufacturing and sustainability of PSCs. Using Google Scholar and existing literature, 60 laboratory-synthesised cells which utilised the nanomaterials in their perovskite compound active layer were selected to be analysed. 4 of these cells used TiO_2 nanomaterials, 11 used MXene-based nanomaterials, 11 used Graphene-based nanomaterials, 13 used carbon quantum dots, and 21 used carbon nanotubes.

To analyse the influence of the nanomaterials on the efficiency of the PSCs, key performance characteristics of each cell were identified. These characteristics included power conversion efficiency (PCE), current density (J_{SC}),, outer-circuit voltage (V_{OC}), and fill factor (FF). Once these metrics were determined, an average was calculated for each nanomaterial additive and communicated using visual means such as bar graphs, as shown below in Figure _. This allowed for one to easily recognise which nanomaterial was the best performing in each of the metrics. These findings and visuals are extracted from my final research report.

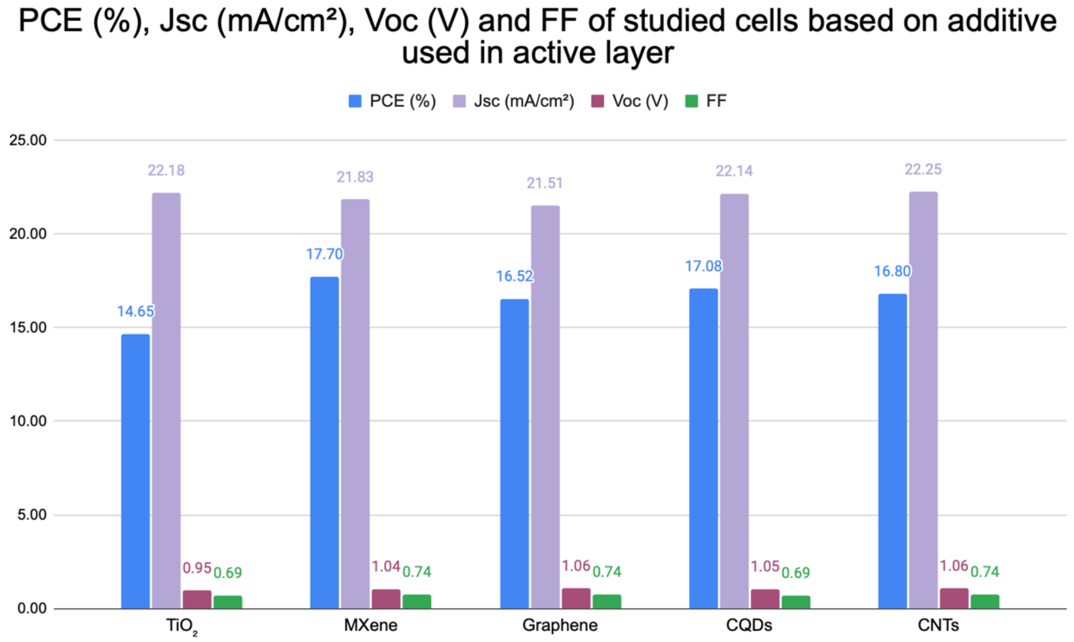


Figure _: Comparison of nanomaterials' averages of key performance metrics

For stability and durability, the cells were categorised according to the environmental conditions under which they were tested. These conditions include changes in relative humidity (RH), changes in temperature, exposure to light and composition of atmosphere in which the cell is placed. This method of analysis was the most accurate comparison as these variables significantly influence the lifetime of a PSC. From the 60 cells, 3 common conditions were identified and used to classify the cells. These conditions were as follows:

1. Inert atmosphere, ambient conditions, 1 solar illumination
2. Inert atmosphere, ambient temperature, 1 solar illumination, RH controlled
3. Inert atmosphere, ambient temperature, no light exposure, RH > 0%

These findings were recorded and communicated using tables. An example of some of the findings that were communicated in the final report are shown in Table 1 below.

Condition 1: Inert atmosphere, ambient conditions, 1 solar illumination

Active layer composition	**Nanomaterial additive**	**Initial PCE retained (%)**	**Duration (h) / Days**	**Study**
$MAPbI_3{:}TiO_2$	TiO_2	95 – 99	1 920 / 80	(Yang *et al.*, 2019)
$CsFAMA{:}CNT{:}TiO_2$	$CNT{:}TiO_2$	80	144 / 6	(Jin *et al.*, 2022)
$CsPbI_3/Ti_3C_2T_x$	$Ti_3C_2T_x$	85	2 400 / 100	(Chen *et al.*, 2020)
$MAPbI_3 + AGQDs$	$Graphene$	89	960 / 40	(Kadhim, Mohammad and Abd Ali, 2022)
$CH_3NH_3Br + PbI_2 + CH(NH_2)_2Br + CsI + PbBr_2 + DMSO + DMF$	$CQDs$	90.1	240 / 10	(Alkahtani *et al.*, 2022)
$(FAPbI_3)_{0.95}(MAPbBr_3)_{0.05}$	$CQDs$	83	1 000 / 42	(Liu *et al.*, no date)
$MAPbI_3 + CNT - PAA - S$	$CNTs$	80	1400 / 58	(Wang *et al.*, 2022)

Table 1: Performance of studied in cells in inert atmosphere, ambient conditions under constant 1 solar illumination.

When analysing whether the inclusion of nanomaterials would help PSCs be manufactured on a large-scale basis, one needs to determine the overall cost of the nanomaterial's synthesis, as well as the cost of the method of integrating the nanomaterial into the active layer itself. If these 2 factors proved to be high cost, manufacturers and producers of PSCs will have difficulty justifying the material's usage. In addition to this, an increased cost of these 2 factors will in turn increase the individual cost of the PSC itself, reducing the accessibility of the panels within the solar PV market and thus prohibiting its widespread expansion.

The overall cost of each nanomaterial was calculated by researching existing nanomaterial products synthesised by companies such as Nanografi, ACS Materials, and Merck and creating an average price per milligram. When possible, the synthesis method was also recorded. This was then communicated in table form as shown below in Table 2. Please note that 'CVD' in Table 2 is an abbreviation for Chemical Vapour Deposition.

Manufactured nanomaterials and costs on Merck, ACS Materials, and Nanografi

Additive	Form	Company	Product number	Synthesis method	Cost per sample (€)	Cost per mg (€)	Average cost per additive (€/mg)
TiO_2	Nanotube	Merck	799289	Not provided	334 / 500 mg	0.67	**0.45**
TiO_2	Nanopowder	Merck	637254	Not provided	186 / 50 g	0.004	
TiO_2	Nanowires	Merck	774529	Not provided	337 / 500 mg	0.67	
$Ti_3C_2T_x$	Few layer	Merck	924962	Etching	531 / 500 mg	1.06	**1.02**
$Ti_3C_2T_x$	Few layer nanoflakes	ACS Materials	MXTF01A5	Etching	788.90* / 500 mg	1.58	
$Ti_3C_2T_x$	Multilayer nanoflakes	ACS Materials	MXTM0101	Etching	428.88* / 1 g	0.43	
Graphene	QD	Merck	900726	Not provided	133 / 50 mg	2.66	**0.68**
Graphene	GO, paste, non-exfoliated	Merck	900704	Not provided	190 / 25 g	0.01	
Graphene	rGO	Merck	806579	Not provided	436 / 500 mg	0.87	
Graphene	N-doped GO, 1 mg / mL	Merck	791520	Not provided	331 / 25 g	0.01	
Graphene	Single layer	ACS Materials	GN1P0005	Thermal exfoliation reduction, Hummer's method	139.47* / 500 mg	0.28	
Graphene	Single layer, research grade	ACS Materials	GNP1F005	Thermal exfoliation reduction, Hummer's method	505.59 / 5 g	0.51	

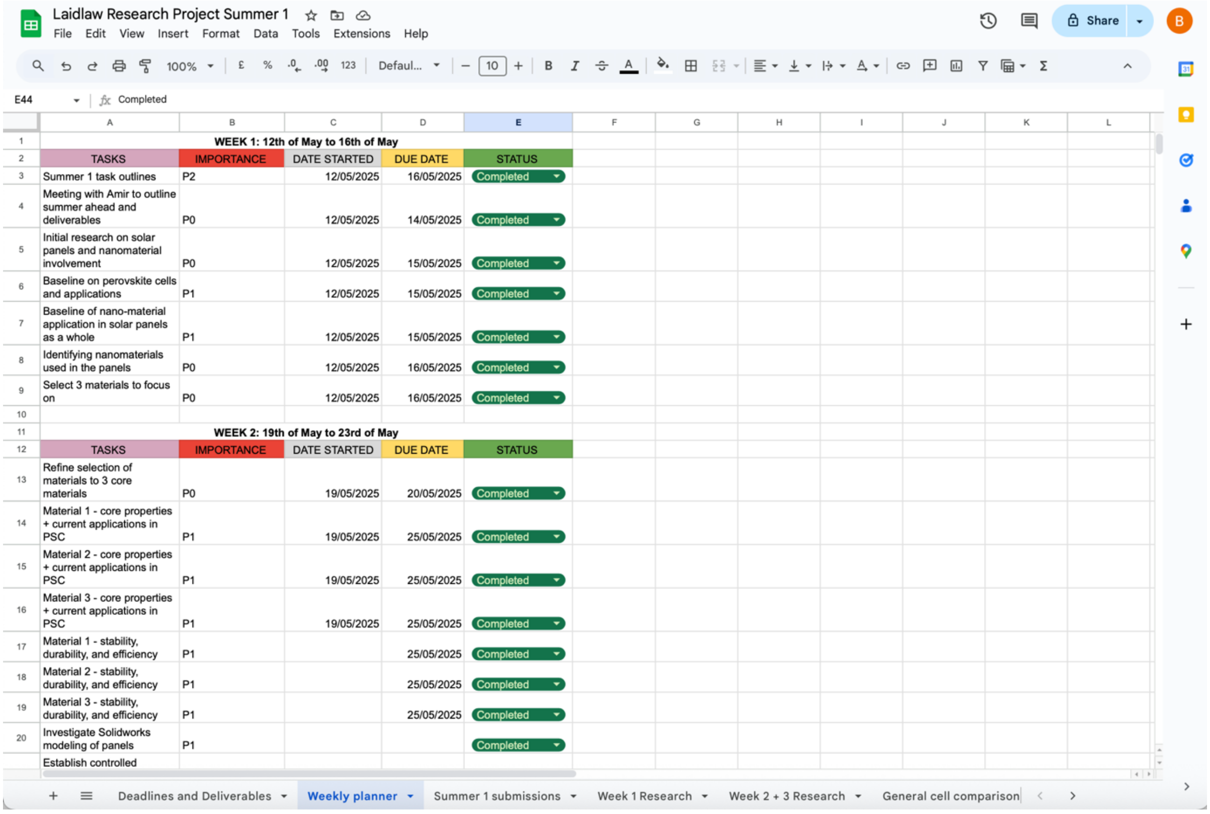
Graphene	Hydroxyl functionalised	ACS Materials	GNPOH0A5	CVD	209.21 / 500 mg	0.42	
CNT	SWCNT	Merck	773735	Not provided	747 / 250 mg	2.99	**0.62**
CNT	SWCNT, highly purified (1 - 2 nm diameter)	ACS Materials	CSH11901	CVD	350.43* / 1 g	0.35	
CNT	SWCNT, highly purified (< 2 nm diameter)	ACS Materials	CSH001A5	CVD	287.67* / 500 mg	0.57	
CNT	SWCNT, industrial grade	ACS Materials	CSI11101	CVD	167.37* / 1 g	0.17	
CNT	MWCNT	Merck	698849-1G	Not provided	208 / 1 g	0.21	
CNT	MWCNT, highly purified (10 – 20 nm diameter)	ACS Materials	CMP20105	CVD	120.30* / 5 g	0.02	
CNT	MWCNT, highly purified (> 50 nm diameter)	ACS Materials	CMP40111	CVD	104.61* / 10 g	0.01	
CQDs	Water soluble, 420 ± 10 nm	Nanografi	NG10QD0949	Not provided	480 / 50 mg	9.6	**6.40**
CQDs	Water soluble, 590 - 620 nm	Nanografi	NG10QD0979	Not provided	45 / 25 g	0.0018	
CQDs	Water soluble, 420 ± 10 nm	Nanografi	NG10QD0952	Not provided	480 / 50 mg	9.6	

Table 2: Market value of nanomaterial additives on mainstream chemical suppliers such as Merck and Nanografi (ACS Materials, 2025; Nanografi, 2025; Sigma Aldrich, 2025).

**Converted from $ to € using exchange rate on 19/06/2025 for simplicity of comparison*

Lastly, the sustainability footprint of the selected nanomaterials was determined using Life Cycle Assessments (LCAs) from literature. LCAs are extremely useful in showing a breakdown of the environmental impacts of a product from initial production to its afterlife, as well as showing which processes are potentially the most harmful. Aspects such as greenhouse gas emissions (GHGs), ecotoxicity, acidification, recyclability, and electricity consumption were analysed and compared. Furthermore, additional research was conducted into whether the nanomaterial when used in the active layer could decrease instances of lead leakage.

To keep on schedule, Google Sheets was used to keep track of the necessary tasks each week and to ensure that deadlines were met. In addition to this, Google Sheets was also used to record findings from literature, as well as calculate key metrics.



WEEK 1: 12th of May to 16th of May

TASKS	IMPORTANCE	DATE STARTED	DUE DATE	STATUS
Summer 1 task outlines	P2	12/05/2025	16/05/2025	Completed
Meeting with Amir to outline summer ahead and deliverables	P0	12/05/2025	14/05/2025	Completed
Initial research on solar panels and nanomaterial involvement	P0	12/05/2025	15/05/2025	Completed
Baseline on perovskite cells and applications	P1	12/05/2025	15/05/2025	Completed
Baseline of nano-material application in solar panels as a whole	P1	12/05/2025	15/05/2025	Completed
Identifying nanomaterials used in the panels	P0	12/05/2025	16/05/2025	Completed
Select 3 materials to focus on	P0	12/05/2025	16/05/2025	Completed

WEEK 2: 19th of May to 23rd of May

TASKS	IMPORTANCE	DATE STARTED	DUE DATE	STATUS
Refine selection of materials to 3 core materials	P0	19/05/2025	20/05/2025	Completed
Material 1 - core properties + current applications in PSC	P1	19/05/2025	25/05/2025	Completed
Material 2 - core properties + current applications in PSC	P1	19/05/2025	25/05/2025	Completed
Material 3 - core properties + current applications in PSC	P1	19/05/2025	25/05/2025	Completed
Material 1 - stability, durability, and efficiency	P1		25/05/2025	Completed
Material 2 - stability, durability, and efficiency	P1		25/05/2025	Completed
Material 3 - stability, durability, and efficiency	P1		25/05/2025	Completed
Investigate Solidworks modeling of panels	P1			Completed
Establish controlled				

Figure x: Google Sheets system used to keep track of tasks and deadlines, as well as record research findings

3. Research findings

The results of this research provide an extremely interesting and useful insight on the influence of nanomaterials within PSCs, as well as their overall environmental impact. In addition to this, one concluded that there was no nanomaterial that championed every category analysed. For example, MXene nanomaterials such as $Ti_3C_2T_x$ and V_2CT_x achieved the highest PCE, current density and fill factor results, making them the best performing nanomaterial from an efficiency perspective. In addition to this, PSCs utilising MXene in its active was shown to outperform the other nanomaterials and retain substantial levels of PCE under various environmental conditions, demonstrating its ability to enhance the cell's stability and durability in realistic scenarios. However, TiO_2 was found to be the most inexpensive nanomaterial additive to synthesise, followed by Graphene and CNTs. Overall, one found concerning environmental impacts associated with the life cycles of all of the nanomaterials, calling into question the current methods of production and manufacturing. One positive from a sustainability perspective was that MXene, CNTs, and CQDs were shown to help reduce occurrences of lead leakage within the active layer, addressing a key concern of PSCs. These findings demonstrate the ability of nanomaterials to enhance the strengths of PSCs, as well as rectify some of the fundamental issues of PSCs.

4. **Reflection on research project**

This research project has been an incredible opportunity to improve and grow critical skills such as research methods, report and article writing, and project planning. The self-run nature of the project, whilst working with a leading expert in the field such as Dr. Amir Pakdel, gave me the ability to take ownership and accountability of the research and its findings, as well as learn an immense amount of knowledge. Working with Dr. Pakdel has been a huge privilege and has allowed me to explore the world of nanomaterials extensively. Furthermore, his guidance and advice helped me refine and improve the final research report into a piece of academic literature in which I take pride. It has also allowed me to develop a new research topic, in which I will be exploring the life cycle assessments of the nanomaterials analysed and if implemented into PSCs, how would their life cycles and outcomes change.

Although I initially planned to work in Dr. Pakdel's laboratory and construct the individual cells to test the influence of the specified nanomaterials, restrictions on use of laboratory equipment and training, as well as the period over which the project had to be completed resulted in a change to a complete literature review. Whilst this presented itself as a challenge at the time, it became an opportunity to refine my research and analysis skills, as well as use crucial software such as Microsoft Excel and Google Sheets.

Overall, I am extremely proud of the results I have managed to achieve with this project and the findings of the research itself. Not only did this project allow me to grow in confidence as a researcher, but it also enabled me to discover new interests and immerse myself in the world of renewable energy and nanomaterials. I look forward to being able to take these skills and knowledge into the rest of the programme, my degree, and career beyond Trinity.

5. **References**

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