An Undergraduate Thesis Proposal

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This thesis proposal, tentatively titled as "***Improvement of Optical Confinement for the Perovskite Solar Cell***" has been submitted under the supervision of Dr. Mahmud Abdul Matin Bhuiyan, Professor of the Department of Electrical and Electronic Engineering at Chittagong University of Engineering and Technology, Chattogram.

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1. Tentative Title

Improvement of Optical Confinement for the Perovskite Solar Cell.

2. Introduction

2.1 Background Study

Addressing the global power crisis, we have seen the demand for power becoming increasingly critical where the failure of supply of adequate power bringing severely adverse implications. Factors such as pandemics, geopolitical conflicts, Europe's sudden transition, depleted global inventories, and climate uncertainties have collectively exerted immense pressure on energy markets worldwide. With global unrests escalating each day, the flow of fossil fuel have been hindered by regional conflicts and political turmoil which makes it an urgent need to lessen the dependency on them and rely more on naturally found renewable sources. Also, burning these resources has resulted in alarming levels of pollution, causing substantial environmental harm. The adverse effects of this pollution have compelled the world to redesign the strategies of power generation, reminding us the significance for renewable energy solutions. Among all the renewable sources, Solar photovoltaic (PV) technology, in particular, has seen a remarkable 82% cost reduction from 2010 to 2019, according to the International Renewable Energy Agency (IRENA) [1]. With the progression of research, we have seen different types of solar cells emerging such as Crystalline Silicon (c-Si) Cells, Thin-Film Solar cell, Organic Cell, Perovskite Solar Cell, Dye-Sensitized Solar Cells (DSSC) or Grätzel cells, Multijunction Cells, Tandem Cells, Quantum Dot Solar Cells, Organic-Inorganic Hybrid Solar Cells and so on. Among all these emerging options, perovskite solar cells are gaining attractions due to their efficiency gains, rapid advancements and versatility.

2.2 Perovskite Solar Cell

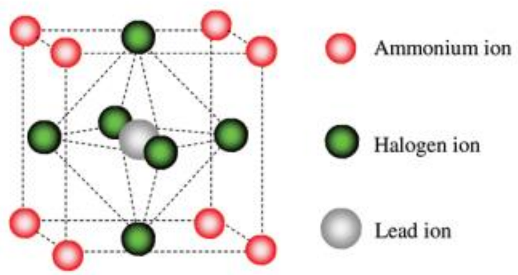

Figure 1: Crystal structures of perovskite compounds [2]

Perovskite solar cells are based on a crystalline structure known as perovskite, named after the Russian mineralogist Lev Perovski. Their unique crystal lattice, comprising organic and inorganic components, enables them to absorb sunlight efficiently and convert it into electricity. In just over a decade since their discovery as a photovoltaic material, perovskite solar cells have witnessed unprecedented progress, surpassing the efficiency records of traditional solar technologies. To the best of our knowledge, incorporation of Perovskite started back in 2009 in a work done by Kojima A. et. al. [3] where the photovoltaic performance of $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$, organic-inorganic lead halide perovskite compounds was investigated as visible-light sensitizers in photoelectrochemical cells. These perovskite materials possess distinctive optical properties, excitonic properties, and electrical conductivity, apart from being derived from abundant sources such as lead, carbon, nitrogen, and halogens. The researchers studied the photovoltaic function of perovskite nanocrystalline particles, which are spontaneously arranged on TiO2 as n-type semiconductors and found cells to have 3.13% and 3.81% efficiency for $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$ respectively.

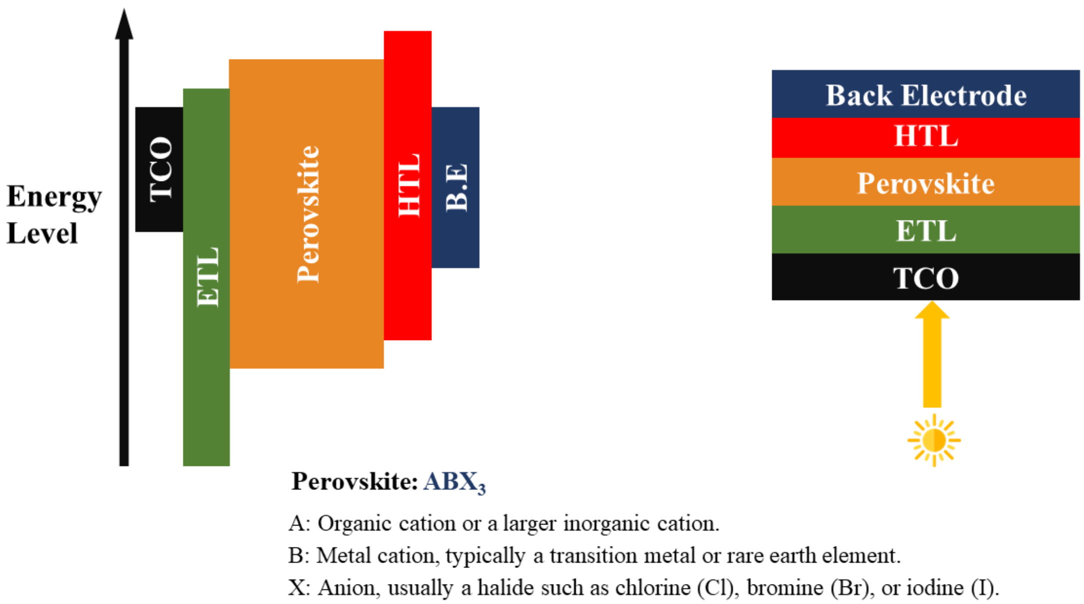

Figure 2: General structure of Perovskite Solar Cell

2.3 Literature Review

Remarkable progress has been witnessed in the performance of Perovskite cells. Reported in the year 2009, methylammonium lead halide ($CH_3NH_3PbX_3$, X = Cl, Br, I) based Perovskite Solar Cells had just 3.8% of efficiency reported by Kojima A. et. al. [3] where now we can see PeSC going well above 24% [4]. Among the published works so far, researchers have achieved efficiency of 24.35% with Jsc of 25.60mA/cm^2 [5]. Optical confinement can boost the short circuit current limit by absorbing more light in the absorber layer. Various techniques are available to boost the Jsc and efficiency of perovskite solar cell. According to Troung et al. [6] introducing a top antireflection front electrode (p-ARFE) which is made of fiber arrays that can boost the Jsc to 20.2 mA/cm^2 which 6.3% greater than planner one. Right choice of Anti-Reflective front electrode, highly reflective back contact and introduction of light scattering system in between absorber layer and back contact can improve Jsc limit [7]. Besides

IBC structured back electrode and cost-effective antireflection coating using printable mesoporous SiO2, efficiency can be enhanced in perovskite solar cell [8]. To increase the optical confinement on cell performance, Wei et. al. [9] cited various types of light manipulation techniques including aperiodic arrays, plasmonic scattering, nanoparticle, microlens array, optical cavities. Tooghi et. al. [10] also reported that there are other structural aspects such as tuning perovskite absorbent, device architectural manipulation or side layer materials adjustment. Bringing changes in the solar cell design and well-studied integration of nanostructures hold the key to significantly enhance solar cell efficiency by employing various effective light-trapping mechanisms [11]–[14]. Even adopting advanced lithography techniques, precisely tuned energy bands or engineered interfaces - a considerable amount of emitted light remains unabsorbed within the solar cell. Researchers opined for two possible causes behind this which are (a) obstruction of light penetration due to reflection (b) solar energy is not exclusively absorbed by the active layer alone, but non-active layers also end up absorbing some energy [15].

Table 1: Summary of Foundational works for Optical Confinement

Ref.	Cell	Optical Confinement Methods Used	Examined Samples	Outcome	
				Jsc*	Efficiency
[7]	ZnO:Al/ZnO/CdS/ CIGS/interfacial layer/Mo/glass	Anti-reflection at front Interfaces (Air/Glass).	Thick Layer	+ 4.4%	
			Thin Layer	+ 4.4%	
		Highly reflective at back contact (ZrN).	Thick Layer	+ 1.6%	
			Thin Layer	+ 8.1%	
		Light scattering between absorber and back contact.	Thick Layer	+ 1.7%	
			Thin Layer	+ 17.8%	
		Light Management by semi-ellipsoidal texture.	Thin Layer	+ 22%	
[9]	ITO/PEDOT:PSS/ $CH_3NH_3PbI_3{-}xClx$/ PCBM/Bphen/Ag	Moth-eye nanostructures incorporation with metal back electrode.	Flat	19.16	14.2%
			Grating	20.76	15.4%
			Moth-eye	21.9	16.3%
[16]	glass/Ag/AZO/Ag NPs/ AZO/n-a Si:H/ i-a Si:H/ p-a SiC:H	Plasmonic back reflector designed with silver nanoparticle arrays randomly placed.	Flat n-i-p	13.1	6.3%
			Plasmonic n-i-p	15.1	7.9%
			Textured n-i-p	14.8	7.8%
			Textured p-i-n	17.4	11.1%
[10]	ITO/TiO2/Perovskit e/ CuSCN/Back Contact	Nanostructured PSC with plasmonic enhancement	Planar cell	18.54	15.1%
			Modified Cell (with varied curvature)	23.4	21%

[6]	ITO/TiO2/ $CH_3NH_3PbI_3$:P3HT: Al	Atop antireflection electrode based on dielectric fiber arrays	Plain and Fiber arrayed top layer (varied fiber radius, spacing and angular incidence)	+ 6.3%	
[17]	ITO/PEDOT:PSS/ Perovskite/ ZnO/ Ag	Spheroid Ag nanoparticle (np) at back	Without np	18.57	16.66%
			Spheroid np (e=0)	21.36	18.21%
			Spheroid np (e=.75)	22.94	21.58%
			Spheroid np (e=.89)	23.88	22.92%
			Spheroid np (e=.92)	16.15	13.26%
[18]	ITO/TiO_2/$MASnI_3$/ Spiro-OmeTAD/Au	Incorporation of ZrN/SiO2 shell nanoparticles in the active layer.	Planar	27	12.9%
			ZrN/SiO2 (90nm)	34.5	16.9%
			ZrN/SiO2 (115nm)	40.3	20%

*For the short-circuited current density, J_{sc} column, if the values have '+' sign infront of them, it indicates increase from the base value. If there's no sign at the beginning, it refers to the Jsc value in mA/cm^2

Table 2: Studied Optical Confinement Techniques

Category	Techniques
Front Surface	Moth Eye Texture
	Top Antireflection Front Electrode (p-ARFE)
Back Surface	Highly Reflective Back Contact
	Plasmonic Scattering
Intermediate Layer	Light Scattering Layers
	Aperiodic Arrays
	Microlens Arrays
	Optical Cavities
Material and Absorption Enhancement	Spherical Structures
	Nanoparticle Integration
	Tuning Perovskite Absorbent
	Device Architectural Manipulation

3. Objectives

1. Examine the optical confinement techniques for Perovskite Solar Cell.
2. Compare among the confinement techniques that have already been studied.
3. Propose a confinement method for improved Power Conversion Efficiency (PCE).

4. Methodology

To prepare the workflow and methodological steps, we have classified the works in the following steps to achieve the objectives we have claimed to reach at. The flowchart below shows our working steps diagram.

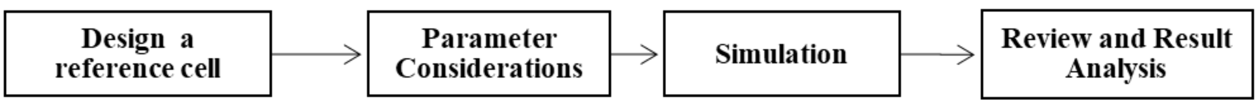

Figure 3: Methodology Flowchart

4.1 Design a reference cell

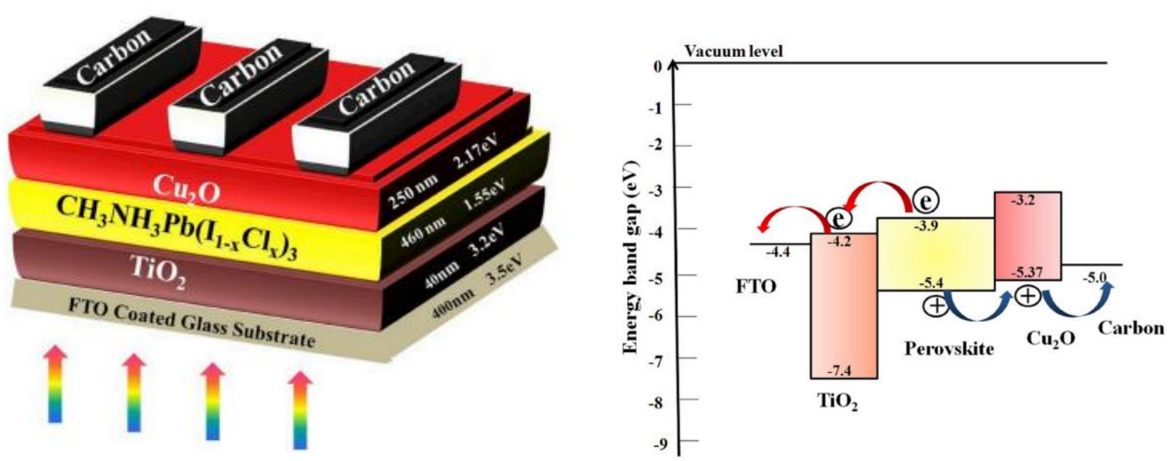

Figure 4: Cell Structure and Band Diagram of the designed Cell [19]

Based on the works of Rai S. et. al. [19] we have simulated Glass/FTO/TiO2/CH3NH3Pb(I1-xClx)3/Cu2O/Carbon solar cell on SCAPS 1D for benchmarking purposes. The values provided in the paper had been used while designing the solar cell. The J-V curve along with the other simulation data have also been shared below.

Table 3: Data table comparing the data found from the literature and our simulation

Parameters	From Literature	From Experiment	From Simulation
Voc (V)	1.15	1.11	1.14
Jsc (mA/cm^2)	23.34	22.3	23.27
FF (%)	70.31	74.5	73.25
PCE (%)	18.92	18.4	19.49

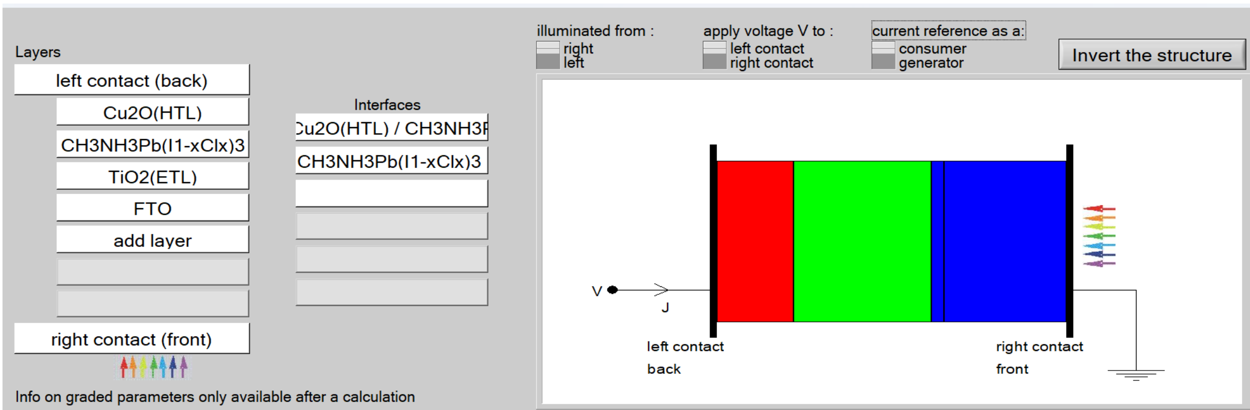

Figure 5: Cell Definition Panel from SCAPS 1D

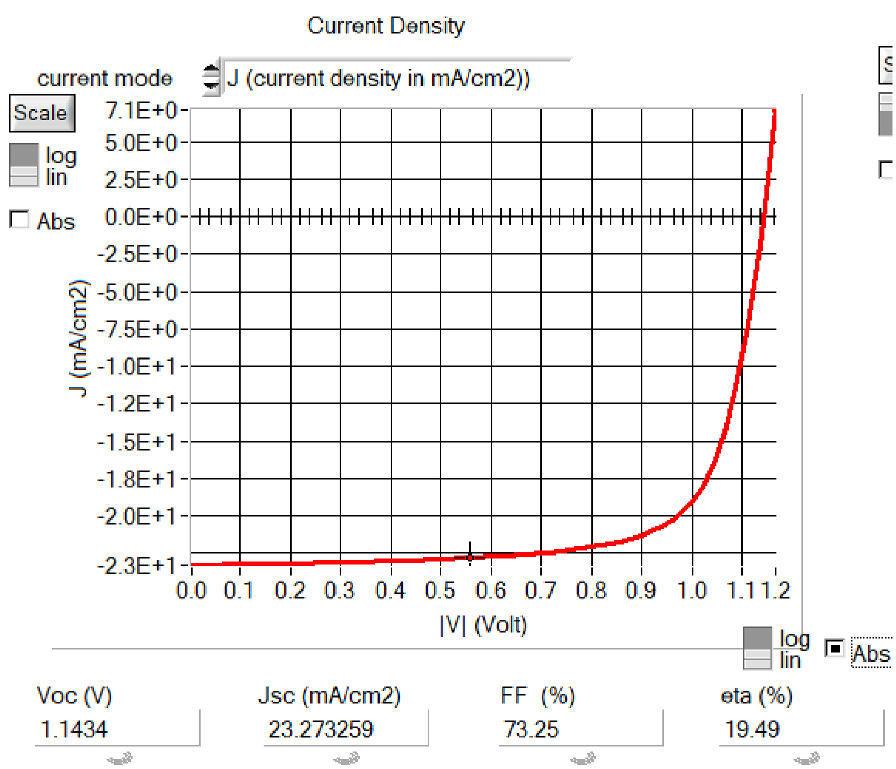

Figure 6: Simulation Result including J-V Curve

4.2 Parameter Considerations

Table 4: Parameters to Consider

Optical	Electrical
Reflection coefficient	Short Circuited Current density (Jsc)
Refraction coefficient	Fill Factor (FF)
Absorption	Power Conversion Efficiency (PCE)
Haze	
Angular Independent Diffusion (AID)	
Scattering	
Optical Path	

4.3 Simulation

There are numerous software available for solar cell simulation and performance analysis related works i.e. Silvaco, Scaps 1D, WxAMPS, Ansys Lumerical, Comsol Multiphysics, SunShine etc. Looking at the scale and scope of the work, we plan to execute the simulations on Lumerical. Considering the timeline and scope of this work, initially we plan to individually simulate the following techniques.

- Anti-reflection coating layer.
- Spheroid Ag nanoparticle at the back.
- Atop antireflection electrode based on dielectric fiber arrays

We will be analyzing the performance indicating parameters and optimize them accordingly.

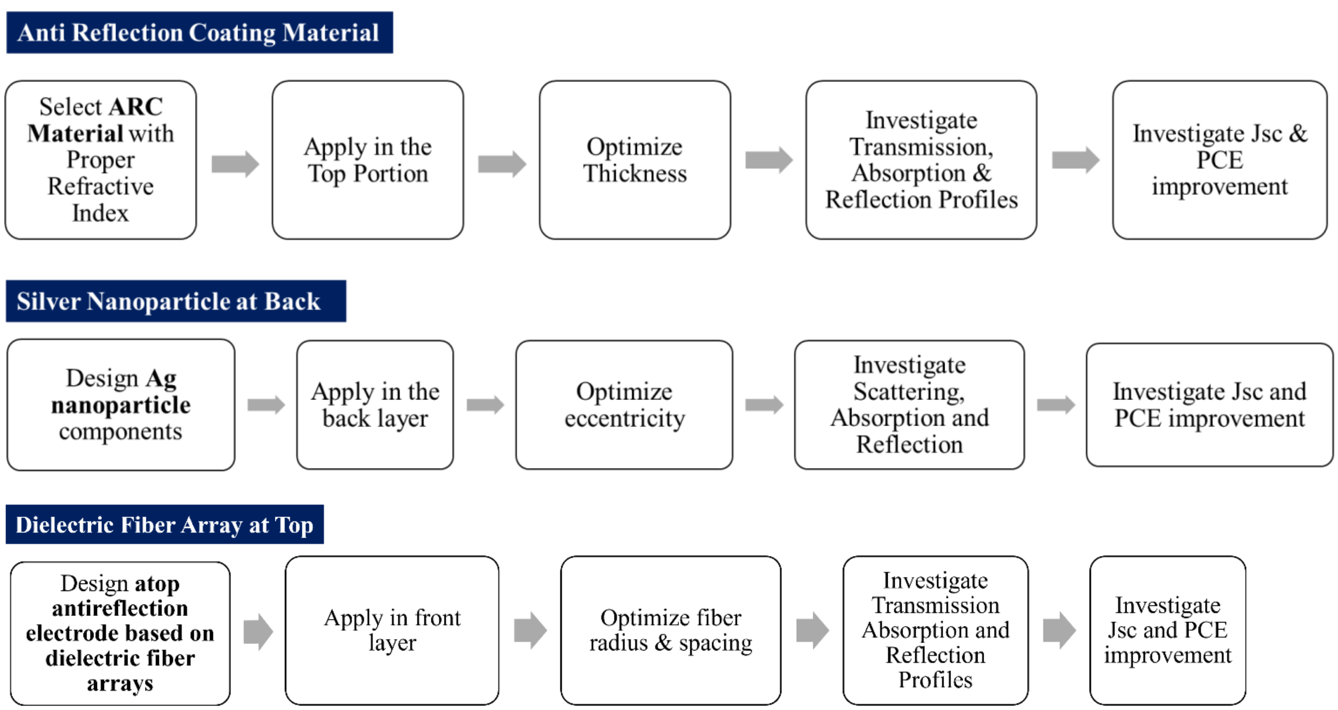

Figure 7: Methodological approaches for Simulation

4.4 Result Analysis and Review

Evaluate performance on other cells and investigate if it can be established as a generalized technique. The sole purpose of this phase is to design methods to be implemented in different perovskite cells and generate enhanced performance as we expect to reach the following accomplishments.

- Detailed analysis and provide recommendation on the selection of optical confinement methods for upcoming research works.
- Increased Jsc and Efficiency for Perovskite Solar cell.
- Develop generalized or semi-generalized method for optical confinement.

5. Progress & Timeline

			L-4 T-1				L-4 T-2			
Task	**Completion**		**May 23**	**June 23**	**July 23**	**Aug 23**	**Sept 23**	**Oct 23**	**Nov 23**	**Dec 23**
Preliminary Investigations and Planning	**92%**									
Reviewing Current Research Landscape	95%									
Identifying Research Gaps	90%									
Defining Research Objectives and Scope	90%									
Literature Review & Theoretical Foundation	**70%**									
Conducting a Comprehensive Literature Review	60%									
Brainstorm on Possible Solutions	60%									
Selecting Major Parameters	90%									
Methodology	**43%**									
Developing the Research Methodology	60%									
Collecting Cell Design Parameters	20%									
Select Simulation Software	50%									
Simulation	**3%**									
Learning to Use Lumerical FDTD	10%									
Benchmarking and Result Optimization	0%									
Designing Cells with Various Confinements	0%									
Analyzing Simulation Results	0%									
Results and Conclusion	**0%**									
Presenting Research Findings	0%									
Providing In-depth Discussion of Key Results	0%									
Performing Comparative Analysis with Literature	0%									
Interpreting Findings in Relation to Objectives	0%									
Evaluating the Applicability for General Case	0%									

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