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I hereby declare that this thesis, entitled **"FABRICATION AND CHARACTERIZATION OF PEROVSKITE SOLAR CELLS AND PERFORMANCE ANALYSIS USING THEORETICAL STUDY,"** is a genuine record of research conducted by me under the supervision and guidance of **Dr. Suman Chatterjee**, Professor, Department of Physics, University of North Bengal, West Bengal. This work is submitted for the award of the degree of **Doctor of Philosophy** in **Physics**. I also affirm that no part of this thesis has been previously submitted for the award of any other degree or diploma at any other university. Additionally, this thesis has been thoroughly checked for originality using Drillbit plagiarism detection software.

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This is to certify that the thesis titled **"FABRICATION AND CHARACTERIZATION OF PEROVSKITE SOLAR CELLS AND PERFORMANCE ANALYSIS USING THEORETICAL STUDY"** is an original piece of research work carried out by **Mr. Joy Sarkar** under my supervision and guidance at the **Department of Physics**, University of North Bengal, West Bengal. This submission is for the degree of **Doctor of Philosophy** in **Physics**. I also confirm that no part of this thesis has been previously submitted for any other degree or diploma at any other institution.

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This thesis is dedicated to my family, especially my mother, Archana Sarkar, my brother, Jayanta Sarkar, and in loving memory of my father Joydeb Chandra Sarkar

Preface

Photovoltaic technologies have emerged as a forefront research area in the quest for sustainable energy solutions. As one of the most potent renewable alternatives to fossil fuels, photovoltaics offers the promise of clean, abundant energy through the direct conversion of solar radiation into electricity. While conventional silicon-based solar cells have demonstrated significant potential in harnessing solar energy, their high costs with complex fabrication methods have hindered widespread adoption and competitiveness with traditional power generation methods. In contrast, perovskite solar cells (PSCs) have captivated the scientific community and industry with their remarkable characteristics. These non-conventional photovoltaic technologies stand out due to their exceptional power conversion efficiencies, cost-effectiveness, and the use of recyclable materials. This thesis, titled "**FABRICATION AND CHARACTERIZATION OF PEROVSKITE SOLAR CELLS AND PERFORMANCE ANALYSIS USING THEORETICAL STUDY**," delves into the innovative landscape of PSCs. It investigates the complex procedures of fabricating these cells, rigorously evaluates their performance through detailed characterization, and employs theoretical models to uncover insights that drive further advancements in this field.

This thesis is structured into several key sections. **Chapter 1** offers a comprehensive review of existing literature, emphasizing current developments and challenges in the advancement of perovskite solar cells. This chapter also explores various generations of photovoltaic technology, providing a brief introduction to the components and working principles of perovskite solar cells. **Chapter 2** outlines the theory and working of the various experimental techniques employed to characterize the several components that comprise perovskite solar cells. **Chapter 3** provides an in-depth exploration of the theoretical frameworks and modeling tools utilized to analyze and interpret the performance of perovskite solar cells. **Chapter 4** explores a novel fabrication technique for enhancing the device performance of $CH_3NH_3SnI_3$-based perovskite solar cells, focusing on the strategic utilization of a DMSO and activated carbon powder mixture as a counter electrode. **Chapter 5** theoretically examines the impact of Br-substitution on band gap broadening, followed by a detailed theoretical

analysis (based on DFT and SCAPS-1D modeling) of the device performance of lead-free inorganic Ge-based perovskite solar cells. **Chapter 6** studied the effect of metal (Cr, Sr, Ag, and Cu) doping on the performance of all-inorganic Sn-based perovskite solar cells theoretically. **Chapter 7** provides a comprehensive exploration of the fabrication and characterization methods employed to investigate the performance of $CsSnI_3/CsSnBr_3$ heterostructure perovskite solar cells. The experimental findings are substantiated through theoretical analysis utilizing Density Functional Theory (DFT). Finally, the essential findings of this study have been outlined in **Chapter 8**.

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Joy Sarkar

List of Abbreviations and Symbols

CB	Conduction band
PSC	Perovskite Solar cell
DSSC	Dye-sensitized solar cell
EDS	Energy-dispersive X-ray spectroscopy
Eg	Energy band-gap
EIS	Electrochemical Impedance Spectroscopy
FF	Fill Factor
FTO	Fluorine doped Tin oxide
FWHM	Full width at half maximum
HOMO	Highest occupied molecular orbital
Imax	Maximum current
Isc	Short-circuit current
ITO	Indium tin oxide
JCPDS	Joint committee on powder diffraction standards
Jsc	Short-circuit current density
LUMO	Lowest unoccupied molecular orbital
PEDOT	[poly(3,4-ethylenedioxythiophene)]
Pmax	Maximum power
PV	Photovoltaic
Pt	Platinum

R_S	Series resistance
R_{Sh}	Shunt resistance
SEM	Scanning electron microscopy
TCO	Transparent conducting oxide
V_{max}	Maximum voltage
V_{OC}	Open circuit voltage
XRD	X-ray diffraction
η	Power conversion efficiency
λ_{max}	Maximum absorption wavelength.
FTIR	Fourier Transform Infrared Spectroscopy
PL	Photoluminescence Spectroscopy
KPFM	Kelvin Probe Force Microscopy
AFM	Atomic Force Microscopy
XPS	X-Ray Photoelectron Spectroscopy
UPS	Ultraviolet Photoelectron Spectroscopy
m_e	Effective mass of electrons
m_h	Effective mass of holes
ΔH_f	Formation enthalpy
A	Electron affinity
χ	Electronegativity
R_y	Rydberg energy constant
ε_s	Static dielectric constant

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