SYNTHESIS, CHARACTERIZATION, AND ANALYSIS OF LEAD-FREE INORGANIC PEROVSKITE FOR SOLAR CELL APPLICATION

BELLO, OLUWASEYI OLUWATIMILEYIN

19PCE02037

OCTOBER, 2021

SYNTHESIS, CHARACTERIZATION, AND ANALYSIS OF LEAD-FREE INORGANIC PEROVSKITE FOR SOLAR CELL APPLICATION

BY

BELLO, OLUWASEYI OLUWATIMILEYIN
19PCE02037

A DISSERTATION SUBMITTED TO THE SCHOOL OF POSTGRADUATE STUDIES IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE AWARD OF MASTER OF SCIENCE (M.Sc) INDUSTRIAL PHYSICS (RENEWABLE ENERGY AND MATERIAL SCIENCE) IN THE PHYSICS DEPARTMENT, COVENANT UNIVERSITY, OTA, OGUN STATE, NIGERIA.

OCTOBER, 2021

ACCEPTANCE

This is to attest that this research work is accepted in partial fulfillment of the requirements for the award of the degree of Master of Science (M.Sc) in Industrial Physics (Renewable Energy) in the Department of Physics, College of Science and Technology, Covenant University, Ota, Nigeria.

Mr. John A. Philip ……..

(Secretary, School of Postgraduate Studies) Signature and Date

Prof. Akan B. Williams ……..

(Dean, School of Postgraduate Studies) Signature and Date

DECLARATION

I, BELLO, OLUWASEYI OLUWATIMILEYIN (MATRIC NO: 19PCE02037) declare that this research was carried out by me under the supervision of Dr. Moses E. Emetere of the Department of Physics, College of Science and Technology, Covenant University, Ota, Nigeria. I attest that this dissertation has not been presented wholly or partially for the award of any degree elsewhere. All sources of data and scholarly information used in this dissertation are duly acknowledged.

BELLO OLUWASEYI OLUWATIMILEYIN ……

Signature and Date

CERTIFICATION

We certify that this project titled **"SYNTHESIS, CHARACTERIZATION, AND ANALYSIS OF LEAD-FREE INORGANIC PEROVSKITE FOR SOLAR CELL APPLICATION"** is an original research work carried out by BELLO, OLUWASEYI OLUWATIMILEYIN (19PCE02037) in the Department of Physics, College of Science and Technology, Covenant University, Ota, Nigeria under the supervision of DR. MOSES E. EMETERE. We have examined and found this work acceptable as part of the requirements for the award of the degree of Master of Science in Industrial Physics (Renewable Energy and Material Science).

Dr. Moses E. Emetere ……..

(Supervisor) Signature and Date

Prof. Mojisola R. Usikalu ……..

(Head, Physics Department) Signature and Date

Prof. Elijah O. Oyeyemi ……..

(External Examiner) Signature and Date

Prof. Akan B. Williams ……..

(Dean, School of Postgraduate Studies) Signature and Date

DEDICATION

This research is dedicated to God. I am grateful to Him for his help throughout this programme.

ACKNOWLEDGEMENTS

I give God the glory and adoration for giving me life, strength, and the impetus to start and forge on with my studies. I appreciate the Chancellor, Covenant University, Bishop David Oyedepo and the entire board of regents. I appreciate the Vice-Chancellor and the entire management team of Covenant University. I am very grateful to Professor Akan B. Williams, Dean of the School of Postgraduate Studies, Dr. Emmanuel O. Amoo, Sub-dean of the School of Postgraduate Studies, and Professor Temidayo V. Omotosho, Dean of the College of Science and Technology for their selfless effort. I wish to express my profound gratitude and appreciation to my Head of Department, Professor Mojisola R. Usikalu and former Head of Department, Professor Ahzegbobor P. Aizebeokhai, for their constructive criticisms, contributions, enthusiastic encouragements, reassurances of faith, useful and timely suggestions throughout the successful completion of study.

I am deeply grateful to my supervisor, Dr. Moses E. Emetere, without whose expertise, kindness, advice, and unyielding support, I would not have been able to complete this research work. I appreciate my family, especially my mother, sister, aunts and uncles, and grandfather, who have provided the monetary resources for this academic program. None of this would have started or continued without their support and encouragement. My heartfelt gratitude also goes to Professor M. L. Akinyemi and Dr. Maxwell Omeje for their help and encouragement during this whole program. I am grateful to the Department of Petroleum Engineering and the Department of Chemical Engineering for their permission to use their labs for this research work. I appreciate Engineer Bolujo, Engineer Daramola, Engineer Adegbite, and Mr Adeyemi for their help and expertise throughout the lab work for this research. I thank the Physics Laboratory of the Department of Physics, who provided much of the beakers for the synthesis carried out in this research. I also thank Professor Marc Burgelman for the permission to use his software, SCAPS-1D, for the electrical characterizations in this research. Further appreciation goes to Dr S. A. Akinwunmi, Dr. T. A. Adagunodo, Dr. O. O. Adewoyin, Dr. K. D. Oyeyemi, Pastor Ayara William A, Mr. A. Akinpelu, Mr Arijaje Theophilus, Mr Araka, Mr Ayanbisi, Mrs Morakinyo Ruth, Mrs Okeniyi Elizabeth, Mr Elijah Adewale, and Miss Fasuyi Nifemi. I thank all members of faculty, staff and students, of the Department of Physics, who have in various ways impacted me and contributed to the success of my study.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

ABSTRACT

Perovskites are at the forefront of research into possible replacements for cumbersome and expensive silicon based solar cells. Lead based inorganic and organic-inorganic hybrid perovskite solar cells have been breaking records for efficiency, approaching 25% in recent years. However, these suffer from instability problems along with the possible health hazards in the long term. Hence, there has been a parallel search for lead-free, and preferably inorganic, perovskite solar cells in the hope of matching and ultimately exceeding the achievements of lead perovskite analogues. Based on in-depth literature review, this research proposed that structural modifications of perovskite using stoichiometry, dopants, and additives be used as a unique technique for enhancing the efficiency of lead-free inorganic perovskites. Four inorganic perovskites were synthesized via solution and solid-state reaction methods with several additives (such as plant extracts and Isopropanol) and dopants (such as copper and silver). The plants extracts were obtained from *Buxus sempervirens, Cercis Occidentalis, Plecranthus scutellariodes, Kola Nitida, Carica Papaya, Ficus Exasperata, and Musa Paradisiaca*. The optical characterization was carried out using X-ray Fluorescence spectroscopy (XRF), and Ultraviolet-Visible (UV-VIS) spectroscopy. The electronic characterization was performed using SCAPS-1D to obtain Power Conversion Efficiency (PCE), current density, voltage, doping density, flat band potential, and external quantum efficiency (QE). $CaZnBr_3$ had an efficiency of 7.52% at 100 μm, with a band gap of 3.658 eV. As a pure lead-free inorganic perovskite, it is already higher than existing lead-free inorganic perovskites. When *Buxus Sempervirens* extract was added, the efficiency improves to 9.71% at 0.2 g and 9.74% at 0.5 g. $NaCaZn_2Br_6$ had low efficiency because of its low short circuit current density (Jsc), steep Mott Schottky curve, and low QE. $Na_2Zn_2Br_6$ performs better as a double perovskite, with higher efficiency of 8.31% in its pure form than $CaZnBr_3$, with an optimized efficiency of 9.78% when doped with 0.2 g of *Musa paradisiaca* extract. In conclusion, the use of stoichiometry, dopants, and additives for structural modifications of inorganic perovskites has been proposed for obtaining new perovskite candidates and PCE optimization. It is recommended that the novel double perovskite $Na_2Zn_2Br_6$ be researched further using different synthetic routes.

Keywords: Perovskite, Dopants, Characterization, Synthesis, Additives, SCAPS-1D.