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

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

BY

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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.

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#### 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).

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## DEDICATION

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

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#### 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<sub>3</sub> 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<sub>2</sub>Br<sub>6</sub> had low efficiency because of its low short circuit current density (Jsc), steep Mott Schottky curve, and low QE. Na<sub>2</sub>Zn<sub>2</sub>Br<sub>6</sub> performs better as a double perovskite, with higher efficiency of 8.31% in its pure form than CaZnBr<sub>3</sub>, 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<sub>2</sub>Zn<sub>2</sub>Br<sub>6</sub> be researched further using different synthetic routes.

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