MONTE CARLO SIMULATIONS FOR SURFACE SPUTTERING ANALYSIS AND FIRST-PRINCIPLES CALCULATION OF STRUCTURAL AND ELECTRONIC PROPERTIES OF SELECTED PEROVSKITES

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ACCEPTANCE

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

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DECLARATION

I, **AKINPELU AKINWUMI (18PCE01793),** declare that this research was carried out by me under the supervision of Dr. Oluwole E. Oyewande of the Department of Physics, College of Science and Technology, Covenant University, Ota, Nigeria. I attest that this dissertation has not been presented either wholly or partly for the award of any degree anywhere else. All scholarly materials used in the study are duly acknowledged and cited.

AKINPELU, AKINWUMI **Signature and Date**

CERTIFICATION

We certify that this dissertation titled "**MONTE CARLO SIMULATIONS FOR SURFACE SPUTTERING ANALYSIS AND FIRST-PRINCIPLES CALCULATION OF STRUCTURAL AND ELECTRONIC PROPERTIES OF SELECTED PEROVSKITES"** is an original research work carried out by **AKINPELU, AKINWUMI (18PCE017293)** in the Department of Physics, College of Science and Technology, Covenant University, Ota, Ogun State, Nigeria under the supervision of Dr Oluwole E. Oyewande. We have examined and found this work acceptable as part of the requirements for the award of Master of Science in Industrial Physics.

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DEDICATION

This project is dedicated to those individuals who have been adversely affected by epileptic power supply in Nigeria.

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LIST OF ABBREVIATIONS

BCA	Binary Collision Approximation
CIGS	Copper Indium Gallium Selenide Solar
DFT	Density Functional Theorem
DOS	Density of State
ESPRESSO	opEn-Source Package for Research in Electronic Structure, Simulation and Optimization
HOIPs	Hybrid Organic Inorganic Perovskites
IBSS	Ion Beam Surface Sputtering
IHME	Institute of Health Metrics and Evaluation
KMO	Kaisers-Meyer-Olkin
MALI	Methylammonium Lead Iodide
MALB	Methylammonium Lead Bromide
MATB	Methylammonium Tin Bromide
MATI	Methylammonium Tin Iodide
MC	Monte Carlo
PCA	Principal Component Analysis
PCE	Power Conversion Efficiency
PDOS	Projected Density of State
PSC	Perovskite Solar Cell
QE	Quantum Espresso
SRIM	Stopping and Range of Ion in Matter
TDOS	Total Density of State
TRIM	TRansport of Ion in Matter
WHO	World Health Organization

ABSTRACT

Hybrid organic-inorganic perovskites (HOIPs) have become the fastest growing solar technology due to their power conversion efficiency of about 25.2%, competing with the conventional thin-film technology. Although unique and exceptional, instability and toxic behaviour of the perovskite hamper its commercialization. Therefore, this research was carried out to identify the best and less toxic material that can substitute for lead, by performing ion beam surface sputtering analysis of lead and certain lead-free perovskites and calculations of structural and electronic properties. The ion beam surface sputtering was carried out using both transport of ions in matter (TRIM) module and stoppage and range of ion in matter (SRIM) software package. Quantum opEn-Source Package for Research in Electronic Structure, Simulation and Optimization (ESPRESSO) was used to calculate the structural and electronic properties. The sputtering characteristics results showed similar sputtering pattern. The A-site of these perovskites recorded the highest sputter yields, with a maximum sputter yield around 78° ion incidence. Lattice constants, bulk moduli, density of states, projected and total density of states and band gaps results were compared with the experimental and theoretical values; good agreement was obtained. Tin perovskite ($CH_3NH_3SnI_3$) has the highest sputter yields amongst other less toxic perovskites and it has similar electronic structure to lead iodide perovskite ($CH_3NH_3PbI_3$).Therefore, this research suggests that optical properties be investigated to further examine the potential of tin to replace lead for photovoltaic applications.

Keywords: Band Structure; Density Functional Theory; Density of State; Lead-free Perovskite; Sputtering; Tin Perovskite