Application

Call	SARAO Doctoral
Call Start Date	23 May 2024
Call End Date	20 August 2024
Reference	SDOC240621230796
Applicant Name	BENVOLLENS MALULEKE
Email	benvollens456@gmail.com
ID/Passport Number	9904045107087
Race	African
Gender	Male
Citizenship	South African citizen
Organisation	University of the Western Cape
Birth Date	04 April 1999
Date Generated	19 July 2024 16:04

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CV

Personal Profile

Citizenship Status South African citizen	Country Of Birth South Africa
Current Country South Africa	Institution University of the Western Cape
Race African	ID/Passport Number 9904045107087
Identity Type SA ID Number	Gender Male
Identity Document MALULEKE_B_ID .pdf	Is Disabled No

Qualifications/Certifications

Academic Level Honours	Institution University of Limpopo
Study Field BSc Honours	Name Of Degree Diploma BSc honors physics
Highest Qualification No	Completed Yes
Date Obtained 2023-12-15	Fulltime Yes
Distinction Yes	Date of First Registration 2023-02-06
Academic Record/Transcript Benvollens_Accademic Record.pdf	

Academic Level Bachelors	Institution University of Limpopo

Study Field Physics and chemistry	Name Of Degree Diploma BSc Physical sciences
Highest Qualification Yes	Completed Yes
Date Obtained 2022-12-15	Fulltime Yes
Distinction Yes	Date of First Registration 2018-01-01
Academic Record/Transcript Maluleke B academic record.pdf	

Academic Level Masters	Institution University of the Western Cape
Study Field Mathematical sciences	Name Of Degree Diploma Maters of Mathematica Science
Highest Qualification No	Completed No
Fulltime Yes	Distinction N/A
Date of First Registration 2024-02-02	Intended Completion Date 2024-12-01
Qualification Status In Progress	

Career History

Appointed From 2023-02-13	Appointed To 2023-11-01
Career History Type Contract appointment	Is Current No
Is Fulltime Yes	Organisation lab assiatant
Position lab assistant physics	Sector Science Councils and National Research Facilities

Application

Basic Information

Descriptive Title
Accurate prediction of the specific heat capacity of inorganic perovskites is crucial for advancing the science of quantum materials and optimizing their potential applications in various emerging quantum technologies. This project aims to develop an explainable quantum machine learning (QML) model that is suitable for implementation on a quantum computer to predict the specific heat capacity of inorganic perovskites with high precision. By leveraging the principles of quantum computing and machine learning, the proposed QML model will capture complex material properties and interactions that traditional models may overlook. Furthermore, the integration of explainability techniques will provide insights into the underlying factors influencing specific heat capacity, enhancing the interpretability and trustworthiness of the predictions. The outcomes of this research are expected to contribute significantly to the fields of computational materials science and quantum computing, offering a powerful tool for the design and discovery of novel perovskite materials with tailored thermal properties.

Call Grant Year 2025	Funding Years Requested 3

Short Title
Explainable ML Models for Predicting Specific Heat Capacity of Inorganic Perovskites

Institution University of KwaZulu-Natal	

Geographical Area

Current Province Western Cape	District Municipality Mopani District
District Municipality Ba-Phalaborwa Local	Language Xitsonga
Province Limpopo	Province District Limpopo
Province District Mopani District	

Person History

Funding Organisation Institutional Funding	Is Intern No
Organisation Group Current Organization	

Additional Information: Masters/Doctoral

Is Previously Funded No	Research Project End Year 2028

Research Project Start Year 2025	

Application Category - SARAO Doctoral

Is Fulltime Student Yes	Scholarship Applying For NRF-SARAO
Type Of Nrf Sarao Scholarship Doctoral Science	Type Of Scholarship Doctoral

Degree To Be Funded

Current Activity Studying	Department School Department of Physics
Discipline Physics	Discipline Type Default
Does Degree Include Pre Proposal No	Does Previous Financial Support Binding No
Faculty Faculty of Natural Sciences	Has Masters Upgraded To Doctoral No
Is Currently Registered No	Student Number N/A

Academic Achievement

Academic Level Honours	Average Percentage Marks 72%
Name Of Previous Degree BSc Honours Physics	Timeframe Minimum prescribed period + 6 months
Year 2023	

Details of Research

Aims and Objectives

Aims and Objectives

The aim of this doctoral research is to develop and implement explainable machine learning models to predict the correlation between the specific heat capacity and photoconversion efficiency of perovskite materials. Additionally, the research seeks to explore how these relationships can be elucidated using Quantum Machine Learning (QML) models.

Specific objectives are:

1. **QML Model Development:** Design and develop robust machine learning models capable of accurately predicting the specific heat capacity and photoconversion efficiency of perovskite materials based on their intrinsic properties and structural characteristics.
2. **Explainability and Interpretation:** Implement techniques that enhance the interpretability of the machine learning models, ensuring that the predictions and underlying mechanisms are transparent and understandable. This involves identifying key features and patterns that influence the material properties.
3. **Correlation Analysis:** Investigate the quantitative relationships between specific heat capacity and photoconversion efficiency in perovskite materials using the developed machine learning models to uncover underlying trends and dependencies.
4. **QML Integration for Explainability:** Integrate Quantum Machine Learning (QML) approaches into the predictive modeling framework, leveraging the computational advantages of quantum algorithms to improve prediction accuracy and provide deeper insights into the material properties.
5. **Validation and Testing:** Rigorously validate the developed models using experimental data and benchmark them against existing models to ensure their reliability and generalizability across different types of perovskite materials.
6. **Application and Impact:** Demonstrate the practical applications of the developed models in the design and optimization of perovskite materials for high-efficiency photovoltaic devices, highlighting the potential impact on the field of renewable energy.

Potential Impact (Societal and/or Knowledge) of the Research

This research will contribute significantly to the advancement of explainable artificial intelligence in material science and enhance understanding of the fundamental properties of perovskite materials. By achieving the aims, the project will pave the way for the development of more efficient solar energy technologies. It will also offer practical applications in designing and optimizing perovskite materials for high-efficiency photovoltaic devices, which could have a considerable impact on the field of renewable energy.

Original Problem Statement

The accurate prediction of specific heat capacity in inorganic perovskites is essential for advancing our understanding of their thermal properties, which directly impacts their performance in quantum technologies. Traditional computational models often fall short in capturing the complex interactions and intrinsic properties of inorganic perovskites. This research aims to develop an explainable quantum machine learning (QML) model specifically tailored for predicting the specific heat capacity of inorganic perovskites, leveraging quantum computing to handle the complex interactions that classical ML models might miss. The integration of explainability techniques will ensure that the model's predictions are interpretable, providing insights into the factors influencing specific heat capacity, and enhancing the trustworthiness and practical applicability of the predictions.

Financial Need

Income Bracket
Not applicable

Household Contributor

Nothing Captured

Financial Need - Proof Of NSFAS/ISFAP Funding

Academic record/transcript PROOF OF NSFAS.pdf	Is Funding Received Yes

Attachments

Attachment Document Type Supervisor Recommendation	Submission Document Motivation Letter - Benvollens-1.pdf
Attachment Document Type Supporting Documents	Submission Document Benvollens_Academic record.pdf
Attachment Document Type Supporting Documents	Submission Document MALULEKE_B_ID.pdf