RESEARCH PROPOSAL TEMPLATE

CALL FOR RESEARCH PROPOSALS

PART I: GENERAL INFORMATION (*Entire Proposal should not exceed fifteen (15) pages)*

Title and Brief of/on the Project: **From Industrial Waste to Environmental Solution: Zeolite-Based CO_2 Capture Using Coal Fly Ash**

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Research Area(s) to be addressed: **Water, Environment and Energy**

Co-Investigator/s:

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Project Start Date: August 2024 | Project End Date: December 2028

PART II: PROJECT DESCRIPTION

1. **Introduction**

Carbon dioxide (CO_2) is a significant greenhouse gas contributing to global warming and climate change. The increase in CO_2 levels in the Earth's atmosphere, primarily due to the burning of fossil fuels and deforestation, traps more heat from the sun, leading to a rise in global temperatures. This results in significant environmental changes, including extreme weather events, rising sea levels, and disruptions to ecosystems. Reducing atmospheric CO_2 levels is critical for mitigating these effects and limiting global warming to targets set by international agreements, such as the Paris Agreement. Botswana has agreed to report on carbon stocks and reduce greenhouse gas emissions by 15% by 2030, according to the Paris Agreement. This agreement aligns with Sustainable Development Goal 13 (Climate Action), which aims to limit global temperature rise to 1.5°C above pre-industrial levels.

The development of CO_2 capture technologies is at the forefront of scientific research aimed at mitigating climate change, presenting several challenges that require innovative solutions. Among these, enhancing the selectivity and capacity of capture materials is critical. Materials must preferentially adsorb CO_2 over other gases present in the mixture while also maximizing the amount of CO_2 they can hold. Additionally, the energy required for material regeneration is a significant factor; reducing this energy demand is crucial for improving the overall efficiency and cost-effectiveness of the capture process. The chemical and thermal stability of these materials also plays a vital role in ensuring their long-term usability and minimizing operational costs, addressing concerns around material degradation over time. Moreover, scalability and integration into existing infrastructure pose significant challenges, necessitating technologies that can be effectively scaled up and seamlessly integrated into industrial processes.

Zeolites have emerged as a significant breakthrough in this field, owing to their high surface area, tunable pore sizes, and chemical stability, making them excellent candidates for selective CO_2 adsorption. The synthesis of novel zeolites with optimized pore structures and surface chemistries has enhanced CO_2 capture capabilities. Additionally, the creation of hybrid materials, which combine zeolites with other functional materials, has further improved capture efficiency and selectivity. Successful pilot projects have also demonstrated the feasibility of integrating zeolite-based CO_2 capture technologies into industrial settings, marking a significant step forward in process integration.

Despite these advances, several outstanding issues remain in the use of zeolites for CO_2 capture. The economic viability of these technologies, especially when compared to other methods, poses a challenge to widespread adoption. The long-term stability of zeolites and their resistance to fouling by impurities in gas streams are areas needing further improvement. Direct air capture (DAC) efficiency is another critical concern; enhancing the performance of zeolites in DAC, where CO_2 concentrations are significantly lower than in flue gases, requires ongoing research. Additionally, translating laboratory-scale successes to industrial-scale applications involves overcoming considerable engineering and economic hurdles, highlighting the need for continued innovation and research in scaling up these technologies for practical use.

The synthesis of zeolites from coal fly ash (CFA) for CO_2 capture marks a transformative approach to climate change mitigation, ingeniously converting a coal combustion by-product into a valuable asset for carbon sequestration. This method significantly boosts cost-effectiveness by repurposing waste, utilizing the rich silica and alumina content in CFA, and ensuring a scalable supply chain from an abundant waste source. Moreover, the ability to customize zeolite properties optimizes CO_2 capture efficiency, directly reducing operational expenses. Embracing circular economy ideals, this approach, particularly through collaborations with entities like the Morupule Coal Mine and Botswana Power Corporation—key players in energy production and (CFA) generation in Botswana—, not only delivers substantial environmental benefits and assists in meeting regulatory compliance but also paves the way for potential economic incentives. By transforming CFA, a by-product from Botswana Power Corporation's energy production processes, into valuable zeolites for CO_2 capture, this strategy exemplifies a sustainable and scalable response to one of our era's environmental challenges. It represents a pioneering integration of waste management and advanced material science, pointing towards a greener future and strengthening the relationship between industrial operations and environmental sustainability within the context of Botswana's environmental and economic landscape.

Our team has been actively engaged in research centered around the utilization of coal fly ash (CFA), exploring its potential as a source material for synthesizing zeolites, such as Na-X and ZSM-5. This work represents our ongoing commitment to finding sustainable uses for industrial by-products, specifically in the context of environmental remediation and the challenge of CO_2 capture. In line with these efforts, we have recently detailed our process for extracting high-purity silica from CFA in an article published in *ChemistrySelect*[1]. This proposal aims to build upon our existing body of work by furthering our investigation into CFA-derived zeolites and their application in CO_2 capture technologies.

2. Research Objectives and Methodology

The primary objective of our research is to advance the field of CO_2 capture by leveraging the unique properties of zeolites synthesized from CFA, demonstrating their effectiveness and efficiency in capturing CO2 from various sources. In doing so, we aim to:

- **Enhance Environmental Sustainability**: By converting CFA, an abundant waste product, into high-value zeolites, we aim to reduce waste and contribute to cleaner air, aligning with global as well as national sustainability goals.
- **Promote Gender Equity in STEM**: Through the successful involvement and graduation of MSc and PhD students, particularly women, in this research area, we aim to break barriers and foster a more diverse and inclusive scientific community.

To achieve these broad objectives, we have outlined the following specific goals:

Specific Research Objectives

- **Synthesis and Characterization of Zeolites**: Continue the synthesis of zeolites (Na-X, A, and ZSM5) from CFA, ensuring a high degree of purity and structural integrity. This involves detailed characterization of their physicochemical properties using advanced analytical techniques to understand their CO_2 adsorption capacities and mechanisms.
- **Evaluation of CO_2 Capture Efficiency**: Systematically assess the CO_2 capture efficiency of the synthesized zeolites under various environmental and operational conditions, including different temperatures, pressures, and gas compositions. This will help identify the most effective zeolite types and conditions for maximum CO_2 capture.
- **Enhancing Zeolite Adsorbents for CO2 Capture**: Optimize zeolite-based adsorbents for CO_2 capture by developing efficient pelletizing processes, selecting ideal binders, and identifying optimal sizes and shapes for performance. The project will also focus on enhancing the adsorbents' durability in industrial settings.
- **Computational Optimization of Zeolite Structures**: Utilize computational modeling and simulation techniques to explore and optimize the molecular structures of zeolites for enhanced CO_2 adsorption. This objective seeks to identify modifications to the zeolite framework that could improve selectivity and capacity for CO_2.
- **Environmental and Economic Feasibility Assessment**: Conduct a comprehensive analysis of the environmental impact and economic viability of using CFA-derived zeolites for CO_2 capture. This includes lifecycle assessments to evaluate the sustainability of the process and cost-benefit analyses to determine its economic feasibility.

Through these specific objectives, our research endeavors to make a substantial contribution to the field of CO_2 capture technology, while simultaneously addressing the urgent need for more inclusive and equitable participation in STEM disciplines. By achieving these goals, we not only advance scientific understanding and technological innovation but also contribute to the creation of a more sustainable, equitable, and resilient society.

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[1] T. Manyepedza, E. Gaolefufa, I. N. Beas, M. T. Kabomo, B. Modukanele, *ChemistrySelect* 2024, 9, e202305065. https://doi.org/10.1002/slct.202305065

Methodology

To ensure a comprehensive approach to our research on CO_2 capture using zeolites synthesized from coal fly ash (CFA), we propose dividing the work among both MSc and PhD students. This structured division allows for specialized focus areas while encouraging collaboration and knowledge sharing among the team. Each student's project will focus on a distinct aspect of the research, contributing to a holistic understanding and advancement of CO_2 capture technology. We'll reserve 60% of spots in ecological studies for female students. We'll also consider students with disabilities and from remote areas.

Undergraduate students will join the project for data collection, analysis, and manuscript writing. Collaborators will host students for 3-months, rotating to learn from experts. Students will gain knowledge of data techniques, critical thinking, and interpretation skills. These skills will be useful for future research projects.

PhD Projects

PhD Student 1: "Advanced Characterization and Performance Analysis of CFA-Derived Zeolites for CO_2 Capture"

- **Description**: This project focuses on the in-depth characterization of zeolites synthesized from CFA, assessing their physical, chemical, and structural properties. The student will evaluate the performance of these zeolites in CO_2 capture through various adsorption isotherm tests.
- **Methodology**:
  - **Advanced Characterization Techniques:** Beyond basic characterization, this project will apply sophisticated analytical techniques such as TEM (Transmission Electron Microscopy) for detailed morphological analysis and N_2 adsorption-desorption isotherms for precise pore size distribution and surface area measurements. In situ spectroscopy methods, like FTIR (Fourier-Transform Infrared Spectroscopy), will be used to study the interaction between CO_2 and the zeolite surfaces under different conditions.
  - **Adsorption Performance Testing**: Kinetic adsorption tests will complement equilibrium isotherm studies to evaluate the rate of CO_2 uptake by the zeolites. Temperature-Programmed Desorption (TPD) experiments will be conducted to understand the thermal stability of adsorbed CO_2 and the regenerability of the zeolite materials.

PhD Student 2: "Computational Modeling for Optimizing the Structure of CFA-Derived Zeolites for Enhanced CO_2 Adsorption"

- **Description**: This project aims to use computational methods to model and optimize the pore structure and surface chemistry of CFA-derived zeolites for improved CO_2 adsorption efficiency.
- **Methodology**:
  - **High-Throughput Computational Screening:** This approach will involve screening a large database of hypothetical zeolite structures using computational simulations to predict their CO_2 adsorption properties. The screening will prioritize structures with high surface areas, optimal pore sizes, and functional groups that enhance CO_2 interaction.
  - **Material Optimization and Design:** Utilizing insights from the screening, the project will focus on the rational design of zeolite frameworks, employing DFT to fine-tune the electronic properties of the materials for optimal CO_2 capture. Machine

learning algorithms will be applied to predict the performance of novel zeolite structures, accelerating the design process.

PhD Student 3: " Pelletizing and Form Factor Optimization for Zeolite-Based CO_2 Capture"

- **Description**: This project aims to transform powdered zeolites into pellets or optimized forms to improve industrial usability for CO2 capture. It focuses on developing pelletizing techniques that retain the adsorption properties of zeolites, facilitating easier handling and efficiency in CO2 capture systems.
- **Methodology:**
    - **Binder Selection**: Identify and test binders that effectively agglomerate zeolite powder without compromising CO2 adsorption capacity.
    - **Pellet Size Optimization**: Conduct experiments to determine the optimal pellet size and shape for maximum adsorption efficiency and mechanical stability.
    - **Durability Testing**: Evaluate the structural integrity and adsorption performance of zeolite pellets under cyclic adsorption-desorption conditions to ensure long-term usability.

PhD Student 4: "Evaluating the Environmental Impact and Sustainability of CO_2 Capture Using CFA-Derived Zeolites"

- **Description**: This project assesses the lifecycle environmental impact of utilizing CFA-derived zeolites for CO_2 capture, considering the sustainability of the synthesis process and the overall carbon footprint reduction.
- **Methodology**:
    - **Lifecycle Assessment (LCA):** The LCA will be comprehensive, covering from raw material acquisition (CFA collection) through to the end-of-life of the zeolite material. Critical indicators such as Global Warming Potential (GWP), Acidification Potential (AP), and Eutrophication Potential (EP) will be assessed. Sensitivity analysis will be performed to identify hotspots in the lifecycle where improvements can significantly reduce environmental impacts.
    - **Sustainability Index Development:** A sustainability index specific to CO_2 capture technologies will be developed, incorporating environmental, economic, and social criteria. This index will help in comparing the sustainability of CFA-derived zeolites against other adsorbent materials.

MSc Projects

MSc/Meng/MBA Student 1: "Economic Analysis and Market Potential of CFA-Derived Zeolites in CO_2 Capture Applications"

- **Description**: This project shifts the focus towards the economic aspects of CO_2 capture using CFA-derived zeolites, aiming to assess the market potential and economic viability of this technology. The study will explore cost factors associated with the synthesis and deployment of CFA-derived zeolites, potential revenue streams from CO_2 capture and utilization, and compare these costs and benefits to existing CO_2 capture technologies.
- **Methodology**: The project will employ a cost-benefit analysis framework, incorporating data on material costs, operational efficiencies, and potential market prices for captured CO_2 or secondary products derived from the process. Market analysis methods will be used to identify potential industries and sectors as primary consumers of this technology, evaluating the economic competitiveness of CFA-derived zeolites. Additionally, financial modeling tools will be used to project long-term economic outcomes, factoring in policy incentives,

carbon pricing mechanisms, and scalability considerations.

MSc Project 2: "Evaluating the Impact of Surface Functionalization on CO_2 Adsorption Dynamics of CFA-Derived Zeolites"

Description: This project explores enhancing CO_2 adsorption in CFA-derived zeolites through surface functionalization, focusing on how functional groups affect CO_2 selectivity and adsorption rates. It combines chemical modifications with adsorption testing to find the best strategies for improved CO_2 capture efficiency.

Methodology:

- **Surface Functionalization**: Implement chemical methods to introduce specific functional groups (e.g., amines, silanes) onto the surface of CFA-derived zeolites. Different functionalization agents and conditions (e.g., concentration, reaction time, temperature) will be explored to achieve a range of surface chemistries.
- **Characterization of Functionalized Zeolites**: Utilize Fourier-transform infrared spectroscopy (FTIR) to confirm the presence of functional groups on the zeolite surface. Additional characterization techniques, such as thermogravimetric analysis (TGA) and scanning electron microscopy (SEM), will be used to assess the impact of functionalization on the physical properties of the zeolites.
- **CO_2 Adsorption Experiments**: Conduct adsorption experiments to measure the CO_2 capture performance of the functionalized zeolites. Variables such as pressure, temperature, and gas composition will be adjusted to simulate real-world conditions and assess the performance under various scenarios.

3. Expected Knowledge Outputs and Outcomes

Our endeavor in the synthesis and utilization of coal fly ash (CFA) for the creation of zeolites aimed at CO_2 capture encapsulates a significant stride towards scientific innovation and environmental stewardship. This initiative, underpinned by rigorous academic research and dedication to sustainability, is poised to generate a myriad of knowledge outputs and outcomes, each contributing to the broader objectives of combating climate change and advancing the circular economy. Herein, we delineate the anticipated knowledge outputs and the consequential outcomes expected from this project:

Expected Knowledge Outputs

- **Comprehensive Datasets on Zeolite Characterization and CO_2 Capture Efficiency**: Through meticulous experimentation and analysis, we anticipate compiling extensive datasets detailing the physicochemical properties of synthesized zeolites. This includes their pore size distribution, surface area, adsorption capacities, and selectivity towards CO_2. Parallelly, datasets capturing the efficiency of these zeolites in sequestering CO_2 under various conditions will be developed, offering invaluable insights for optimizing CO_2 capture processes.
- **Optimized Zeolite Structures for CO_2 Adsorption**: Leveraging advanced computational modeling and experimental feedback loops, we aim to identify and refine zeolite structures that exhibit superior performance in CO_2 adsorption. This effort will result in the identification of zeolite modifications that enhance CO_2 selectivity and capacity, potentially setting new benchmarks in the field of carbon capture.
- **Insights into the Environmental and Economic Viability of Using CFA-Derived Zeolites for CO2 Capture**: Integral to this project is the assessment of its sustainability and economic feasibility. We expect to generate comprehensive analyses that weigh the

environmental benefits of diverting CFA from landfills against the energy and costs associated with synthesizing zeolites. Economic assessments will provide a clear picture of the cost-effectiveness of this approach in comparison to conventional CO_2 capture technologies.

- **Establishment of a Scalable, Environmentally Friendly CO_2 Capture Technology**: The culmination of our research efforts is anticipated to be the blueprint for a scalable and eco-friendly CO_2 capture technology. This technology, grounded in the use of waste materials and optimized for efficiency, represents a paradigm shift towards more sustainable industrial practices.

Expected Outcomes

- **Contribution to Climate Change Mitigation**: By enhancing the efficiency and viability of CO_2 capture, this project directly contributes to global efforts to mitigate climate change, aligning with international targets to reduce greenhouse gas emissions.
- **Advancement in the Utilization of Industrial By-Products**: The successful application of CFA, an industrial by-product, in creating value-added materials for environmental applications, underscores the potential of waste-to-resource transformations in contributing to a circular economy.
- **Policy and Industry Implications**: The insights and technologies emanating from this research are expected to inform policy decisions and industrial practices, advocating for the integration of sustainable and cost-effective CO_2 capture solutions in regulatory frameworks and operational strategies.
- **Educational and Social Impact**: Beyond its scientific contributions, this project plays a critical role in educating the next generation of researchers and public stakeholders on the importance of sustainable technologies. By fostering a diverse and inclusive research environment, it also advances gender equity in STEM fields, inspiring broader participation and innovation.
- **Alignment with Pillar 1 of Botswana's Vision 2036:** This project aims to use coal fly ash for zeolite-based CO_2 capture, creating an environmental solution and fostering a knowledge-based economy. It represents a shift towards sustainable manufacturing practices and aligns with Botswana's Vision 2036 goals.

4. Expected Potential Impact of Knowledge Outputs

The expected impact of the knowledge and outcomes generated from our research on synthesizing zeolites from coal fly ash (CFA) for CO_2 capture spans several dimensions, reflecting a profound contribution to environmental science, policy, industry practices, and societal well-being. The multifaceted nature of this project ensures that its impacts are both broad and deep, influencing scientific understanding, technological innovation, environmental sustainability, economic viability, and social equity. Here's an overview of the anticipated impacts:

Scientific and Technological Advancements

- **Innovations in Material Science**: By developing a deeper understanding of zeolite synthesis from CFA and optimizing these materials for CO_2 capture, the project is poised to contribute novel insights to the field of material science. These advancements will expand the knowledge base, potentially leading to new applications of zeolites beyond CO_2 capture, such as in catalysis, separation processes, and pollution control.
- **Enhancement of CO_2 Capture Technologies**: The project's outcomes are expected to significantly improve the efficiency, selectivity, and economic feasibility of CO_2 capture

technologies. This will not only advance the state of the art but also make CO_2 capture more accessible and practical for a wider range of applications, accelerating the adoption of carbon capture and storage (CCS) and carbon capture, utilization, and storage (CCUS) technologies globally.

Environmental Impact

- **Mitigation of Climate Change**: By enabling more efficient CO_2 capture, the project directly contributes to the reduction of greenhouse gas emissions, a critical factor in global efforts to combat climate change. This aligns with international climate goals, such as those outlined in the Paris Agreement as well as Pillar 3 (Sustainable Environment) of Botswana's Vision 2036, and supports the transition to a low-carbon economy.
- **Sustainable Waste Management**: Utilizing CFA, a by-product of coal combustion, in the synthesis of zeolites represents a sustainable approach to waste management. This not only reduces the environmental footprint associated with coal-fired power generation but also contributes to the circular economy by transforming waste into a valuable resource.

Economic and Industrial Benefits

- **Cost Reduction and Economic Viability**: By demonstrating the economic viability of using CFA-derived zeolites for CO_2 capture, the project encourages investment in and adoption of this technology by industries. This can lead to cost savings in CO_2 management and open up new revenue streams through the commercialization of captured CO_2 or the sale of synthesized zeolites.
- **Promotion of Green Industries**: The project supports the growth of green industries, both through the direct application of its research outcomes and by stimulating demand for sustainable technologies. This can foster job creation, economic diversification, and resilience in the face of environmental challenges.

Policy and Regulatory Influence

- **Informed Policymaking**: The knowledge generated from this project provides a robust evidence base for policymakers, potentially influencing regulations, incentives, and standards related to CO_2 emissions, industrial waste management, and environmental protection. This can facilitate the development of policies that encourage sustainable practices and technologies.
- **Global Environmental Governance**: By contributing to the global body of knowledge on CO_2 capture and sustainability, the project can play a role in shaping international discussions and agreements on climate change mitigation, environmental sustainability, and clean technology transfer.

Social and Educational Impact

- **Empowerment through Education**: The project's focus on involving and mentoring students, particularly women and those from underrepresented groups, in cutting-edge research, enhances STEM education and fosters a more diverse and inclusive scientific community. This not only prepares a skilled workforce ready to tackle future challenges but also promotes equity and representation in science, in line with Pillar 2 of Vision 2036 (Human and Social Development).
- **Raising Public Awareness**: Through outreach and dissemination activities, the project raises public awareness about the importance of CO_2 capture and sustainability, encouraging informed public discourse and engagement with environmental issues. This can lead to

increased support for environmental initiatives and policies, driving collective action towards a more sustainable future.

5. Expected Human Capital Contributions

Our project stands as a testament to the successful synthesis and characterization of zeolites from coal fly ash (CFA) for CO_2 capture, reflecting a strong commitment to advancing research and supporting human capital in STEM fields. Notably, we have guided two female MSc students to graduation in this specific area, underscoring our dedication to promoting gender diversity and equity in the scientific community. These accomplishments emphasize our efforts to create an environment that supports and enhances the participation of women in science, contributing valuable perspectives and expertise to the field.

Continuing on this path, we are currently mentoring three final-year undergraduate female students who are exploring the properties and applications of zeolites derived from CFA. This mentorship is a direct reflection of our commitment to nurturing the next generation of scientists and engineers, with a particular focus on encouraging female participation in areas of environmental sustainability and CO_2 capture technologies.

As we pursue funding to further this project, our goal is to provide these promising undergraduate students with opportunities to deepen their research experience and academic careers within this domain. Encouraging them to progress to postgraduate studies as part of our team, we aim to reinforce our commitment to empowering women in STEM. This approach not only supports their professional growth but also ensures the continuity and depth of expertise within our research efforts. Through this sustained mentorship and development, we strive to address global environmental challenges, foster a diverse and inclusive research community, and contribute meaningfully to the advancement of CO_2 capture technology.

6. Research Dissemination/Communication

In our proposal, the dissemination and communication of our findings to the general public and key stakeholders are essential for amplifying the impact of our research on CO_2 capture using zeolites synthesized from coal fly ash. To make our science accessible and engaging, we plan to participate in community-oriented events such as National Science/STEM week, where we can present our work at science fairs and interactive booths. This approach will allow us to directly engage with the general public in a simplified and relatable manner, fostering interest and understanding of the importance of CO_2 capture for environmental sustainability. For key stakeholders, including industry partners, policymakers, and academic peers, our strategy includes targeted workshops, policy briefs, and presentations at scientific conferences, ensuring that detailed, actionable insights are communicated effectively. By tailoring our communication efforts to suit each audience, we aim to build support for and involvement in advancing CO_2 capture technologies, with a strong emphasis on making our research accessible to all through public engagement and stakeholder collaboration. The results from the project will also be published in open-access high-impact factor scientific journals.

7. Research Ethics

Our research project, focusing on the synthesis of zeolites from coal fly ash (CFA) for CO_2 capture, is deeply committed to upholding the highest standards of ethics, inclusivity, and gender sensitivity. This commitment is woven into every aspect of the project, from the conceptualization of the research question to the dissemination of findings and beyond.

Ethical Considerations

We adhere to strict ethical guidelines in conducting our research, ensuring that all experimental procedures are environmentally responsible and sustainable. This includes minimizing waste, using non-toxic materials whenever possible, and ensuring that any waste produced is disposed of in an environmentally friendly manner. We also commit to transparency in our research practices and findings, upholding integrity in data collection, analysis, and reporting. Our ethical stance extends to the treatment of all individuals involved in the project, ensuring fair treatment, respect for privacy, and acknowledgment of contributions.

Inclusivity and Diversity

Recognizing the value of diverse perspectives in enriching research and fostering innovation, we strive to create an inclusive environment that welcomes researchers and participants from all backgrounds. This involves proactive measures to ensure broad representation in our research team, including but not limited to, ethnic, cultural, and socio-economic diversity. We aim to create a workspace that is not only physically accessible but also supportive and welcoming, where all team members feel valued and can thrive.

Gender Sensitivity and Responsiveness

Our project places a strong emphasis on gender sensitivity and responsiveness, acknowledging the historical underrepresentation of women in STEM fields and the importance of gender perspectives in environmental research. We actively seek to recruit female researchers and support their career development, offering mentorship opportunities and fostering a culture that challenges gender stereotypes and biases. In terms of research content, we consider the gendered impacts of climate change and environmental degradation, ensuring that our research questions, methodology, and analysis are sensitive to gender differences and aim to contribute to gender equity. This includes, for example, considering how CO_2 capture technologies can be developed and implemented in ways that are accessible and beneficial to all genders, and ensuring that our dissemination strategies reach and engage a gender-diverse audience.

PART III - COLLABORATIONS

Indications of collaborations within the same institution, between institutions within the country. Collaborations with non-academic partners (private sector and the not-for profit sector) can also be indicated.

Institution	**Contact Person**	**Email address**	**Has the collaborator been approached? Yes/No**	**Role of collaborator**
University of Botswana (Chemistry)	Prof Taye Demissie (M) *Bed Science, MSc Physical Chemistry, PhD Physical Chemistry*	demissiet@ub.ac.bw	Yes	**Computational Modeling** • **Role**: To lead the development and application of computational models aimed at optimizing the structure of CFA-derived zeolites for enhanced CO_2 adsorption. • **Supervisory Responsibilities**: Mentor PhD and MSc students in computational techniques, model development, and data analysis. Provide technical guidance on software use, interpretation of simulation results, and integration of findings into the broader project objectives.
University of Botswana (Environmental Science)	Prof Kebonye Dintwe (M) *BSc Biology, MA Geography, PhD Geography*	dintwek@ub.ac.bw	Yes	**Environmental Studies** • **Role**: To conduct comprehensive LCA studies to evaluate the environmental impact of the entire lifecycle of zeolite-based CO_2 capture technologies, from the extraction of CFA to the end-of-life of the zeolites. This will involve assessing carbon footprint, energy use, and potential environmental benefits. • **Supervisory Responsibilities**: Oversee MSc and/or PhD students undertaking LCA projects, ensuring methodological rigor and alignment with international standards. Assist students in data collection, impact analysis, and reporting.
University of Botswana	Dr Bonang Nkoane (F)	nkonaeb@ub.ac.bw	Yes	**Synthesis and Adsorption Studies**

(Chemistry)	*BEng Chemical Eng, PhD Chemistry*			• **Role**: This collaborator leads the experimental synthesis of zeolites from CFA, focusing on optimizing synthesis protocols to enhance the zeolites' CO_2 adsorption properties. This involves developing new synthesis methods, characterizing the produced materials, and testing their performance in CO_2 capture. • **Supervisory Responsibilities**: Supervision of MSc and PhD students engaged in the synthesis of zeolites. This includes training in laboratory techniques, safety protocols, and data analysis, as well as guiding students in experimental design and interpretation of results.
Botswana International University of Science and Technology	Dr Khaulani Fichani (M) *PhD Natural Resource Economics, MS Mineral Economics, B.ASc. Mining and Mineral Process Engineering*	fichanik@biust.ac.bw	Yes	**Economic Analysis Expert** • **Role**: To perform economic analyses of the zeolite-based CO_2 capture process, including cost-benefit analysis, market potential assessment, and scalability studies. This role is crucial for evaluating the commercial viability of the technology and identifying potential economic incentives. • **Supervisory Responsibilities**: Guide MSc and/or PhD students in economic modeling, analysis of financial data, and interpretation of economic impacts. Help integrate economic considerations with technological and environmental findings.
University of Botswana	Dr Moses Tlhabologo Kabomo (M) *PhD Chemistry (Nanomaterials), MBA, MS Chemistry (Polymer), BSc Chemistry, PRINCE2 Project Management*	kabomotm@ub.ac.bw		**PI, Synthesis and Adsorption Studies** The Principal Investigator (PI) will oversee the project, ensuring coherence across all components and alignment with objectives. The PI will co-supervise students engaged in synthesis, adsorption studies, and pelletizing work, collaborating closely with other collaborators to integrate computational studies, environmental and economic analysis into the research

PART IV - TIME SCHEDULE AND WORK PLAN

Please outline the activities planned for the total period of the project/activity (extend space where required)

Subproject	Activity	Collaborator	Start (Month, Year)	End (Month, Year)
Zeolite Synthesis and Modifications	Advanced characterization of synthesized zeolites	Dr Bonang Nkoane Dr Moses T Kabomo Mr Emmanuel Gaolefufa PhD Student 1	08, 2024	03, 2025
	Post-synthesis modification experiments		04, 2025	09, 2025
	Kinetic and equilibrium adsorption studies		10, 2025	03, 2026
	Optimization of post-synthesis modifications		04, 2026	09, 2026
	Comprehensive data analysis		10, 2026	03, 2027
	Final optimization and performance evaluation		04, 2027	09, 2027
	Integration with other project parts		10, 2027	01, 2028
	Thesis writing and defense preparation		02, 2028	09, 2028
Computational Modelling	Model selection and initial computational setup	Prof T Demissie PhD Student 2	08, 2024	12, 2024
	High-throughput computational screening		01, 2025	06, 2025
	Data analysis and model refinement		07, 2025	12, 2025
	Material optimization and design		01, 2026	06, 2026
	Integration of computational findings with experimental data		07, 2026	12, 2026
	Final analysis and optimization		01, 2027	06, 2027
	Preparation of findings for publication		07, 2027	12, 2027
	Thesis writing and defense preparation		01, 2028	09, 2028
Pelletizing & Form Optimization	Development of pelletizing process	Dr Moses T Kabomo Dr Bonang Nkoane Mr Thapelo Manyepedza PhD Student 3	08, 2024	12, 2024
	Binder selection for stability		01, 2025	06, 2025
	Pellet size and shape optimization		07, 2025	12, 2025
	Durability testing under cyclic conditions		01, 2026	06, 2026
	Integration of pellet optimization findings		07, 2026	12, 2026
	Scale-up feasibility study		01, 2027	06, 2027
	Final optimization and performance evaluation		07, 2027	12, 2027
	Thesis writing and defense preparation		01, 2028	09, 2028
Environmental Analysis (LCA)	Initial literature review on environmental impact	Prof Kebonye Dintwe PhD Student 4	08, 2024	10, 2024
	Training on LCA software and methodologies		11, 2024	01, 2025

	Data collection for LCA		02, 2025	07, 2025
	Execution of LCA study		08, 2025	01, 2026
	Analysis of LCA results		02, 2026	07, 2026
	Integration of LCA findings with project aims		08, 2026	01, 2027
	Advanced LCA studies for optimization		02, 2027	09, 2027
	Final LCA report preparation and review		10, 2027	03, 2028
	Thesis writing and defense preparation		04, 2028	09, 2028
Economic Assessment	Literature review on economic aspects	Dr Khaulani Fichani MSc Student 1	08, 2024	09, 2024
	Training on economic analysis tools		09, 2024	11, 2024
	Data collection for economic analysis		11, 2024	02, 2025
	Execution of economic analysis		02, 2025	06, 2025
	Analysis of economic analysis results		06, 2025	12, 2025
	Integration of economic findings		01, 2026	06, 2026
Post-Synthesis Modifications	Initial literature review and experimental design	Dr Moses T Kabomo Dr Bonang Nkoane MSc Student 2	08, 2024	10, 2024
	Selection and testing of modification techniques		11, 2024	04, 2025
	Adsorption performance testing		05, 2025	08, 2025
	Analysis of modification impact on zeolite properties		09, 2025	12, 2025
	Integration of findings with overall project aims		01, 2026	03, 2026
	Thesis writing and defense preparation		04, 2026	07, 2026