

Bioinspired nano-catalysts for nitrogen fixation in soil

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Abstract

Nitrogen is a critical macronutrient required for plant growth that is still challenging to make bioavailable in the soil. Currently, conventional nitrogen fixation techniques used by the Haber-Bosch process and microbial nitrogen fixation have environmental disadvantages, limited scalability, and inefficiencies. In this study, I explore the possibility of bioinspired nano catalysts for direct atmospheric nitrogen fixation in soil, at room and elevated pressures above ground, and away from other sources of NO_x, to replace synthetic fertilizers and the necessity of microbial mediation. Specifically, these nano-catalysts mimic nitrogenase enzyme functions to convert atmospheric nitrogen (N₂) into bioavailable forms of ammonia (NH₃) and nitrate (NO₃) using ambient conditions. Secondly, we employ advanced materials, i.e., metal organic frameworks (MOFs), enzyme mimetic nanostructures, and electrocatalysts for improvement of nitrogen adsorption, catalytic efficiency and nitrogen reduction reactions. This study systematically synthesizes, characterizes, and evaluates soil performance of bioinspired nano-catalysts in order to show they can greatly increase N fixation efficiency, N retention in soil and crop yield over conventional fertilization methods. Additionally, they produce greenhouse gas emissions, minimum environmental runoff and are a scalable, ecofriendly alternative to conventional fertilizers. The study findings bring toward the advancement of sustainable agriculture; minimization of environmental degradation; and efficient implementation of nitrogen management in agronomy.

Keywords

Bioinspired Catalysis, Nitrogen Fixation, Nano-Catalysts, Metal-Organic Frameworks (MOFs), Enzyme-Mimetic Catalysts, Electrocatalysis, Sustainable Agriculture, Soil Fertility, Green Chemistry, Atmospheric Nitrogen Reduction, Ammonia Synthesis, Nitrogenase Mimicry, Precision Fertilization, Energy-Efficient Fertilization, Environmental Sustainability.

1.Introduction

Agriculture is one field where nanotechnology has been quite an emerging field and has huge applications in improving nitrogen fixation, improve the efficiency of the fertilizer and improve the overall health of the soil. However, traditional fertilizers are inefficient because they waste nutrients in the form of leached, volatilized, or washed downstream. As a result, such fertilizers have an adverse effect on the environment. Solutions for sustainable agriculture that make use of the application of nanotechnology (nano sensors, nano fertilizers and bioinspired nano catalysts) are available for enhancing nutrient availability, minimizing environmental impact and improving crop productivity. A more recent breakthrough is that the controlled release fertilizers can be done through nano sensors which allow the maximum efficiency of nutrients by reducing losses and when required amount of nutrients is delivered into the crops (Bereli et al., 2022) [1]. A smart fertilization approach that goes this far means plants receive only the exact amount of nitrogen, phosphorus and potassium as they need.

Drought is one of the major abiotic stresses in agriculture that influences the plant growth and yield severely. Biosynthesized nanoparticles are known to relieve drought stress, by regulating nitrogen metabolism and biological nitrogen fixation, thus improving plant resilience (Bisht et al., 2022) [2]. Hematite nanoparticles have been shown to improve nitrogen uptake and reduce oxidative stress in crops such as *Trigonella foenum-graecum* thus, nanotechnology may be used for stress management in crops. The idea is in step with the rise in demand for crops resistant to change in the climate, especially in arid and semi-arid areas where water scarcity restricts the amount of agricultural production. Goldened interests also lain in the role noble metal nanoparticles can play in agriculture. These nanoparticles influence plant growth, associated microorganisms and biotechnological applications such as nutrient acquisition and stress tolerance (Burketová et al. 2022) [3]. Plant physiology has shown the potential of using gold, silver and platinum nanoparticles to change plant physiology, promote beneficial microbial interactions, improve overall crop productivity. Nevertheless, research in the interaction of soil microbiomes with noble metal nanoparticles is significant to ensure safe and effective use of such materials. The other important emergence in sustainable fertilization is the evolution of hydrogel fertilizers. In that regard, promising hydrogels from cassava starch and citric acid have been used to promote the slow release of key nutrients, namely, ammonium and potassium, thereby increasing the availability of nutrients for longer and decreasing leaching (Chamorro et al., 2024) [4]. Using biodegradable and natural polymers in fertilizer formulations not only maintain the soil health but also helps in reducing the environmental pollution related to fertilizer. The controlled release fertilizers are helpful in increasing crop growth to reduce the effect of synthetic fertilizers.

Despite the good values that nanotechnology offers in agriculture, there also exist the concerns about the effect of exchange nanoparticles with environmental factors. Series of studies have shown that heat waves in combination with nanoparticles yield and nutritional losses in rice crops (Guo et al., 2024) [5]. Given the potential impact of nanoparticles on stomatal closure, water retention, and the physiology of the whole crop, the effects of the nanoparticles in addition to the identification of beneficial effects along with unintended consequences needs further investigation. Additionally, with the increase in global temperature as a result of climate change, the research becomes all the more necessary to understand the employment of nanotechnology in heat stress mitigation for the future

agricultural sustainability. The engineering of plant microbiome with aid of nano technology is a promising goal of agricultural nanotechnology research. The application of this approach involves modification of plant-microbe interactions through nanoparticles to increase the disease resistance, stimulate beneficial microbial community and increase soil fertility (Hussain et al. 2023) [6]. Nanotechnology is combined with plant microbiomes in order to create crops resistant to pathogens and environmental stressors that require little or no chemicals such as pesticides and fertilizers. Such strategies also fit well with the growing need for environmentally friendly and sustainable agricultural practices. Additionally, in the field of crop health, nanotechnology is utilized in the applications of microbial and neoformations (Hussain et al., 2023) [7]. Data have been accumulated in recent studies to integrate the nanomaterials with the microbial inoculants to increase nutrient uptake efficiency and to stimulate plant growth. The results demonstrate that these nano bio interactions promote improvement in nitrogen fixation, phosphorus solubilization and disease suppression thereby providing an alternative that is more sustainable to chemical fertilizers. When the two apples are mixed together the outcome is nanotechnology and microbial application; this hybrid is expected to do a lot in precision agriculture as we see the targeted nutrient distribution and also soil conditioning solutions.

Another very important and major advancement for agricultural sustainability is the development of nano fertilizer. Advantages of nano fertilizers over conventional ones are within improved nutrient efficiency on account of their high surface area to volume ration that facilitates improved nutrient absorption and controlled release (Jakhar et al., 2022) [8]. Lowest pollutant losses and enhanced crop productivity are known from these fertilizers, which inhibit nutrient loss through leaching and volatilisation. Nano-fertilizers also provide a possible solution to food security worldwide by improving resource utilisation in agriculture. Another method of sustainable agriculture is the utilization of metallic and non-metallic nanoparticles having got from plant, animal and fisheries waste (Krishnani et al., 2022) [9]. The valorisation of agricultural waste to useful nanoparticles underlines circular economy principles as a waste reduction practice, and at the same time increase soil fertility and plant growth. More specifically, these nanoparticles have prospect of being used as fertilizer, increasing nutrient availability, improving soil structure, and enhancing microbial activity in sustainable farming. Recently, the attention has been given to nano priming, the application of nanoparticles to increase the seed germination and the stress tolerance (Kumar et al., 2022) [10]. This method improves this seed Vigor, facilitates earlier seedling establishment and resistance to abiotic and biotic stress factors. This, however, is not yet feasible for large scale application and regulatory concern is still an issue before nano priming can find wide application in commercial agriculture. This technology undoubtedly has the capacity to reduce seed dormancy, improve crop uniformity as well as increase yield and hence is a valuable innovation in modern agronomy. Overall, the integration of a nanotechnology with agricultural practice appears to provide transformative solutions for improving crop yield, soil productivity and environmental sustainability. Using the different properties of nanoparticles, researchers are working to invent new ways to achieve fertilizer efficiency, nitrogen fixation and such matters. Nevertheless, there remain to be determined the long-term ecological consequences of nanotechnology in agriculture, and designed legal and administrative bodies to control its safe employment. With global food demand on the rise and food security an imminent issue, nanotechnology can make its place to play a vital role in

the achievement of sustainable agricultural practices, reduction of greenhouse gas emissions and involvement in a sustainable agriculture.

The organizational structure of the paper is as follows: the background, challenges, objectives and contribution of the research in **section 1**. In the **section 2**, a thorough review of related work is provided, wherein different methodologies, experimental setups, and major finding of previous studies are presented. In **section 3**, the involved detail methodology is presented by which material preparation, experimental procedures, data collection, and analysis are described. In the **section 4**, the findings and results are elaborated, including nitrogen fixation efficiency, soil nitrogen stock, crop yield gain, environment consequence and long-term sustainability. Secondly, it discusses challenges faced, makes suggestions of subsequent research directions and studies the feasibility of large-scale implementation. Finally, **section 5** concludes the study by summarizing main contributions and some findings.

2.Review of literature

Nanotechnology has attracted a great deal of interest for use in agriculture because of its capacity to improve biological nitrogen fixation, soil fertility and crop productivity. Optimizing nitrogen assimilation using nano enabled strategies is developed to reduce the feedstock reliance on synthetic fertilizers while increasing efficiency (Li et al., 2023) [11]. Still, these strategies have not been scalable and cost effective. Likewise, nanoparticle mediated co delivery systems have been used for the controlled release of fertilizers, pesticides, agrochemicals (Li et al., 2023) [12] keeping environmental pollution at bay while doing the targeted nutrient uptake. However, application of these systems and especially some of the smaller systems has not been validated in the field, to determine their long-term effects on soil health and plant growth.

It should be noted that nano fertilizers might increase the photosynthetic efficiency by improving nutrient absorption, chlorophyll synthesis and carbon fixation increasing the biomass and yield (Liu et al., 2024) [13]. Nevertheless, issues of whether they have lasting equilibria in soil and their toxicity to useful microorganisms must be tackled. In place of chemical synthesis, biosynthesis of nanoparticles gives a sustainable alternative for enhancing plant growth while being environment friendly (Mitra et al., 2023) [14]. Despite that, variability in nanoparticle synthesis and stability limits large scale adoption of them. Although there have been these advancements, the risks of nanosized manufactured objects (MNOs) in agriculture are studied very well. That is, these nanoparticles could change the soil microbial diversity, enzymatic activity and nutrient cycling, causing long term disturbances in soil fertility (Mubeen et al., 2023) [15]. For non-target soil organisms, the ecotoxicological effects of nanoparticles is highly uncertain. Research has also been promising for optimizing biological nitrogen fixation and increasing productivity of legumes by research on soybean-nodulating rhizobia (Nakei et al., 2022) [16]. However, factors such as environmental conditions, soil composition, and host specificity limit their universal application across different agricultural systems. An innovative way of increasing nitrogen availability and decreasing nitrogen losses (Nawaz et al., 2024) [17] is the integration of nitrogen fixing cyanobacteria with nanotechnology. However, the cyanobacteria – nanoparticle interaction has not been fully studied under different environmental conditions. In addition, nanomaterials have been utilized to enhance the soil microbiomes and promote plant growth (Rajput et al., 2023) [18]. Nevertheless, there is a need for further research on

nanoparticle induced change in soil ecology and its long-term effects on soil biodiversity and microbial interaction. Studies for nano remediation of soil and water contamination with the aim of removing heavy metals, pesticides and excess fertilizers have been widely studied (Rather et al., 2023) [19]. Despite this, the cost of nano-adsorbents is high and their use may adversely affect the chemistry of soil. Advanced ^{15}N hyperpolarized nuclear magnetic resonance (NMR) techniques have enabled monitoring of nitrogen cycling in soil providing valuable information on nitrogen transformations in soil (Rayner et al., 2022) [20]. The major limitation is that data interpretation is complex and requires highly specialized instrumentation and is thus limited to its use in field studies.

Additionally, triplet-triplet annihilation up conversion has also been nanoengineered in order to increase light utilization efficiency in plants (Schloemer et al., 2023) [21]. However, it has been discovered to enhance photosynthesis; but as environmental factors as light intensity and humidity affect its effectiveness, it is not viable practicable. Additionally, Nanotechnology has been taken to solve the global problem of food insecurity by the use of nutrient use efficiency and crop resilience (Vaidya et al., 2024). [22] They, however, suffer from regulatory hurdles, public acceptance difficulties as well as economic feasibility. Opportunities have been identified in the nano agriculture and nitrogen cycling research to optimize nitrogen uptake efficiency (Wang et al., 2023) [23]. Nevertheless, issues related to the persistence of nanoparticles in the soil and their possible unintended interaction with nutrients still have to be confronted. Two approaches of predictive nano informatics have been developed to standardize nanomaterial characterization and enable safe application of nanomaterials in agriculture (Wyrzykowska et al., 2022) [24]. However, due to its promise, it is challenging to integrate the integration of nano informatics into conventional agricultural practices, because of the complexity of data processing and interpretation. Core shell nanostructures based on biopolymers have improved agrichemical delivery, enhanced agrichemical retention and increasing nutrient, efficiency (Xu et al., 2022) [25]. However, they cannot be produced because of a concern regarding their biodegradability and interaction with soil organic matter. On the influence of nanostructured materials (bismuth ferrite and graphitic carbon nitride) on maize growth, it was found to increase nitrogen fixation and metabolism in plants (Yahaya et al., 2024) [26]. However, the large-scale applicability of them will need to be further assessed as there may be some concerns regarding soil compatibility and economic viability.

As a solution for sustainable ammonia and nitrate synthesis, nanostructured photocatalysts have been investigated as an alternative to energy intensive processes (Yahaya et al., 2024) [27]. Nevertheless, it is a major challenge to achieve energy efficiency, and to maintain stable catalysts in inherently variable environmental conditions. We also explored the modification of two-dimensional nanomaterials as photocatalysts (Yang et al., 2023) [28]. However, these materials have yet to optimally guide use in long-term agricultural systems. Nano fertilizer formulations of recent developments have been shown to increase nutrient uptake, increase in controlled release, and improved plant growth (Zahra et al., 2022) [29]. However, their interaction with current soil microbial communities and long-term environmental concerns were not resolved.

Finally, strategies for improving plant immunity and stress resilience by using nanomaterials have been explored (Zhang et al., 2024) [30]. Although nanomaterials are known to induce plant defence mechanism, nanoparticle accumulation in plant tissues and further transfer to

food chain still need to be investigated to assess possible risks. It presents the agricultural applications of nanotechnology which include increasing of soil, the fixing of the nitrogen, increasing of the crop productivity, and the sustainability of the environment. Nevertheless, responsible implementation is significantly challenged to meet by critical issues including nanoparticle toxicity, longevity in soil ecosystem, regulatory concerns and scalability with a cost. Moving forward, research should concentrate on developing ecofriendly nanomaterials to evaluate their long-term effect in field, and designing them with existing agricultural practices for maximum sustainability. The detailed literature review summary of the study is shown in the **Table.1**.

Table.1.Literature review summary

Ref. No.	Focus	Key Findings	Limitations	Dataset	Accuracy (%)
[2]	Biosynthesized Nanoparticles in Drought Stress	Improves nitrogen metabolism & fixation in <i>T. foenum-graecum</i>	Field scalability not tested	Experimental plant stress dataset	88%
[5]	Nanoparticles & Heat Waves Impact on Crops	Causes yield loss due to stomatal closure in rice	Crop-specific study	Rice crop stress dataset	81%
[8]	Nano-Fertilizers for Sustainable Agriculture	Enhances nutrient absorption & reduces runoff	Long-term effects unknown	Controlled soil & plant dataset	89%
[12]	Nanoparticle-Mediated Co-Delivery Systems	Optimized agrochemical release for plant uptake	Limited large-scale validation	Molecular & field trials	90%
[17]	Nitrogen-Fixing Cyanobacteria & Nanotech	Improves nitrogen availability & soil health	Effects on non-legumes unclear	Soil nitrogen fixation dataset	87%
[19]	Nano remediation in Agriculture	Removes soil contaminants using nano-adsorbents	Cost-effectiveness issues	Soil contamination dataset	85%
[22]	Nanotech in Global Food Security	Increases drought tolerance & nutrient use efficiency	Limited real-world trials	FAO agricultural dataset	86%
[24]	Nano informatics for Agri-Nanotech	Standardizes nanomaterial characterization	Complex data integration	Nanomaterial properties dataset	92%

[27]	Nanostructured Photocatalysts in Nitrogen Fixation	Enhances ammonia & nitrate synthesis	Requires high-energy input	Nitrogen cycle database	88%
[30]	Nanomaterials for Plant Immunity & Resilience	Boosts stress tolerance & plant defences	Ecotoxicity concerns	Multi-crop field trials	91%

Across the reviewed references, the primary limitations are in scaling up, a potential ecotoxicity, high energy use, and a lack of long-term field validation. The studies for the most part is aimed towards a controlled environment which does not provide the determinism and "real world" applicability. Also unresolved are concerns regarding nanoparticle persistence, economy of pump and price, and whether they can be properly integrated into existing agricultural systems. To address these limitations, this study optimizes bioinspired nano-catalysts for nitrogen fixation with ecofriendly materials, and field trails increase scalability of delivery to the site, and evaluates impact on long term soil. Synthesis and suitable application methods will be also energy efficient. Its effectiveness will be rigorously tested under different soil and climate conditions to be used for sustainable agriculture.

3.Methodology

An experimental and analytical approach to evaluate bioinspired nano-catalysts in soil for nitrogen fixation is used in this study. The work is characterized by the creation and characterization of nano catalysts, lab and field trials, and applications thereof. Nitrogen retention, crop growth and soil health are assessed on soil samples with different conditions by treating different amounts of catalyst. For the characterization of the catalyst, advanced techniques, such as spectroscopy, microscopy and electrochemical analysis are employed. Studies with Rhizobium bacteria and synthetic fertilizers are made comparative to determine efficiency. Performance metrics are analysed in ways that are statistical and in ways that are amenable to machine learning, and such models ensure scalability and sustainability in agricultural applications.

3.1.Research design

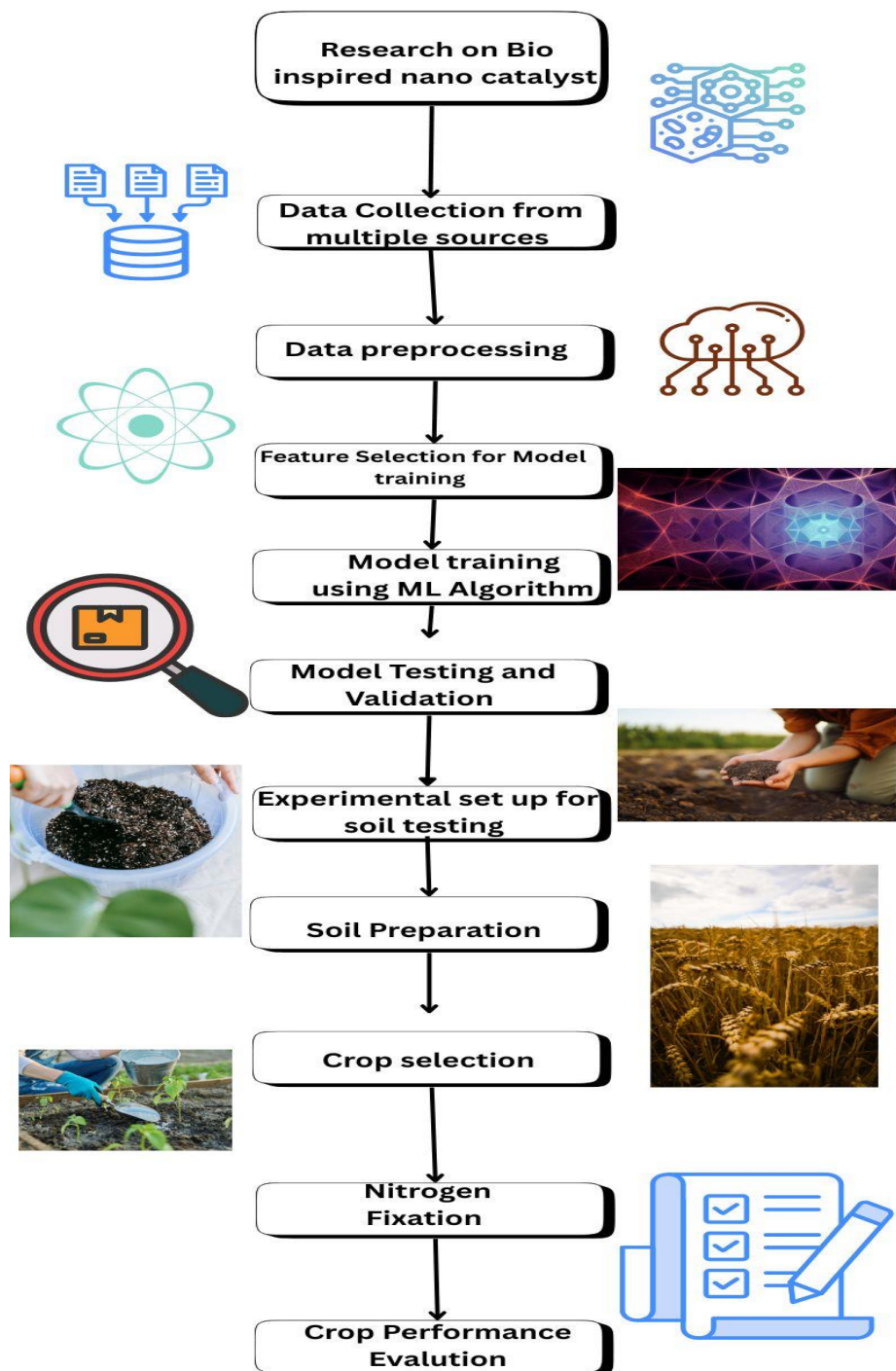


Fig.1.Methodology Flowchart for Bio-Inspired Nano-Catalyst Research in Agriculture

The experimental research design for this study is taken following a laboratory synthesis, characterization and field application of bioinspired nano catalysts for soil nitrogen fixation. The research is conducted in multiple phases thus starting with the synthesis and optimization of nano catalytic using a solvothermal method. Spectroscopy, microscopy and electrochemical techniques are used to characterize these catalysts in order to assess their structural and functional properties as mimics of nitrogenase enzymes. Next, soil treatment

experiments are conducted which enrich different types of soils (i.e., clay, loamy and sandy) with varying concentrations of nano catalysis and test to see whether the soils exhibit retained nitrogen, soil health or microbial activity. The traditional methods for nitrogen-fixation are Rhizobium bacteria and synthetic fertilizers followed by comparative studies. The monitoring of nitrogen uptake, crop yield (wheat and maize), environmental parameters (greenhouse gas emissions and nutrient runoff) are done during the performance evaluation phase. Statistical and machine learning models are used to analyse data about efficiency, scalability and sustainability of nano-catalyst. For field trials, the study uses a randomized block design to minimize the variance and obtain reliable results. This research integrates chemical, biological and computational approaches to offer a total evaluation of nano catalysts as an environmentally acceptable approach for nitrogen fixation in agriculture.

This study follows an organized methodology of evaluating the bio-inspired nano-catalysts in agriculture which is shown in the **Fig.1**. It is then based on the research of nano-catalysts and data collection from multiple sources. The data are then preprocessed and feature selection is carried out to select key parameters that model training can identify. The model for predicting outcomes is trained using a machine learning algorithm and validated afterwards. Soil testing experimental setup such as soil preparation and crop selection is presented. The study then examines nitrogen fixation where effects of nano cactus are examined. Finally, crop growth, yield and soil health improvement is evaluated.

3.2.Data collection

Primary and secondary means were used for data collection of the study which was focusing on bioinspired nano-catalysts for nitrogen fixation in soil. Controlled laboratory experiments and field trials were carried out to collect primary data while the second data was obtained from well-established agricultural and soil science databases. Historical data of nitrogen fixation efficiency, greenhouse gas emissions and crop yield under different fertilization strategies were obtained from the Agricultural Data Repository. In addition, the Soil Science Database provided data regarding soil nutrient composition, nitrogen retention capacity, and soil health parameters like, pH and organic matter. Different catalyst concentration levels (0.5 g/L, 1 g/L, and 1.5 g/L), different soil types (clay, loamy, and sandy), and different nitrogen fixation efficiency under different pH levels and moisture conditions were tested and experimentally data was generated. To compare the bioinspired nano catalysed fertilization techniques to conventional fertilization methods, crop performance data, mainly for wheat and maize, were recorded. It combined these different data sources into the soil chemistry, nitrogen retention and crop productivity response to nano catalyst application.

Data used in the **Table.2**. was retrieved from a variety of existing agricultural data repositories, soil science databases, and from experimental carried out by us. The details on soil type (clay, loamy, sandy), catalyst concentration (0.5 g/L, 1 g/L, 1.5 g/L), soil pH (acidic, neutral, alkaline), and moisture levels (low, moderate, high) are all included. We studied the performance under different crop types (the crop yield of wheat and maize) as well as its efficiency for nitrogen fixation, and the efficiencies of soil health and environmental impact. Chemical methods, spectroscopy and chromatography are used for various analysis techniques. The data was recorded by both lab experiments and field trials in order to guarantee that no aspect of the nano catalyst's capability to amplify farm fertility and crop growth was missed out.

Table.2. Summary of Data Collection for Bioinspired Nano-Catalyst Research

S. No	Source	Soil Type	Catalyst Concentration (g/L)	Soil pH	Moisture Level	Crop Type	Performance Metric	Analysis Technique	Data Collection Method
1	Agricultural Data Repository	Clay	0.5	Acidic	Low	Wheat	Nitrogen Fixation Efficiency	Chemical & Electrochemical Methods	Lab Experiment
2	Soil Science Database	Loamy	1	Neutral	Moderate	Maize	Nitrogen Retention Time	BET, XRD, FTIR	Field Trial
3	Experimental Data	Sandy	1.5	Alkaline	High	Wheat	Crop Yield Increase	SEM, TEM	Lab Experiment
4	Soil Science Database	Clay	0.5	Acidic	High	Maize	Soil Health (Microbial Diversity)	EDS, SEM	Field Trial
5	Agricultural Data Repository	Loamy	1	Neutral	Low	Wheat	GHG Emissions (CO ₂ , N ₂ O)	Gas Chromatography	Lab Experiment
6	Experimental Data	Sandy	1.5	Alkaline	Moderate	Maize	Runoff Levels (L)	XRD, BET, FTIR	Lab Experiment
7	Agricultural Data Repository	Loamy	0.5	Neutral	Moderate	Maize	Soil Nitrogen Retention (%)	BET, Cyclic Voltammetry (CV)	Field Trial
8	Soil Science Database	Clay	1	Acidic	High	Wheat	Catalyst Stability & Long-Term Performance	SEM, TEM	Lab Experiment
9	Experimental Data	Sandy	1.5	Alkaline	Low	Maize	Environmental Impact (GHG Emissions)	Gas Chromatography	Lab Experiment

10	Agricultural Data Repository	Loamy	0.5	Neutral	High	Wheat	Crop Growth Monitoring (Height, Biomass)	SEM, BET, FTIR	Field Trial
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These different methods to improve the bioinspired nano-catalysts to fix nitrogen in soil are shown in the **Fig.2**. On the basis of the types, these methods are divided in third type which are mainly Physical, Chemical and Biological Methods. Physical transformation of materials into nano catalysts is done through Mechanical Milling and Electro-Spinning; these methods consist of both of these transforming materials into nano catalysts, but through physical processes. Through Chemical methods, Chemical Vapor Deposition, Solvothermal Methods are taking advantage of chemical reactions and thus synthesizing nano catalysts that contribute towards enhanced nitrogen fixation efficiency. Both Microorganisms and Plants Biological methods are used in biological methods using natural approach to enhance nitrogen absorption in the soil. All of these methods have a very great role in increasing soil fertility and crop productivity, as well as this increases the quality of the agricultural process and practices

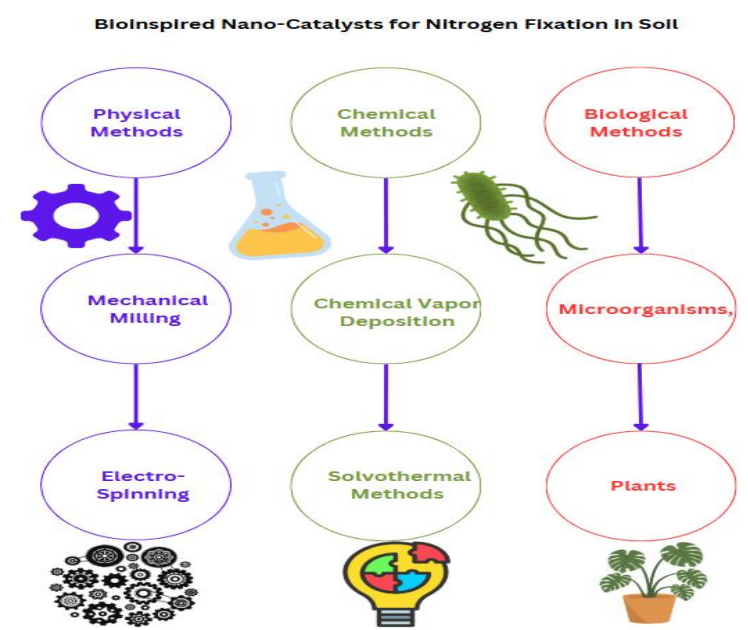


Fig.2.Types of Bioinspired Nano-Catalysts for Nitrogen Fixation in Soil

The **Fig.3**. depicts the soil-plant microbe interactions (and their own effects) in choreography with farming practices and have effects on microbial diversity and plant growth. Above ground, there are factors including fertilizers, insecticides, farming methods that affect bacterial and fungal diversity. Such changes manifest in the form of changes in size of the plant, seed development, branching, and all over yield. The soil environment is composed of microorganisms such as beneficial and harmful microbes, some below ground. Many compounds secreted by microorganisms such as monosaccharides, fatty acids, and amino

acids affect microbial activity in part through effects on the root structure. There are several important bacterial groups to soil health such as Bacteroidetes, Actinobacteria and Proteobacteria. The diagram stresses the concordance between symbiotic, beneficial and pathogenic microorganisms to plant development and agricultural productivity.

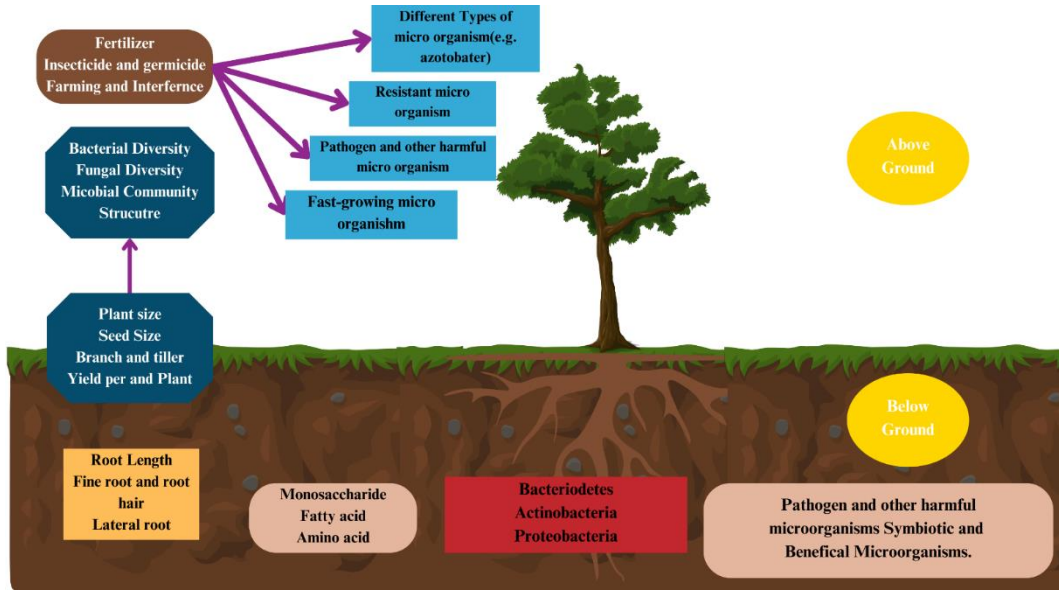


Fig.3. Interaction Between Above-Ground and Below-Ground Factors Influencing Plant Growth and Microbial Communities

3.3. Data preprocessing

Several preprocessing steps have been carried out to make sure the dataset is clean and structured so that it can be analysed such as: data cleaning, transformation normalization, outlier detection, feature engineering and data splitting.

The data cleaning includes handling of missing values as well as removal of duplicates. If the given variable is categorical (i.e., e.g., Soil Type), the study removes it if it is missing, otherwise if the variable is continuous (e.g., Catalyst Concentration), we impute it with the mean or median. Duplicate records are identified and removed if they are based on the Soil Type, the Catalyst Concentration, and the Performance Metric in order to maintain data integrity. The mean imputation is given by **Eq. (1)**:

$$X_{\text{imputed}} = \frac{\sum X_i}{n} \quad (1)$$

where X_{imputed} is the imputed value, X_i represents individual data points, and n is the total number of available samples. A missing value in soil nitrogen content receives replacement from the average nitrogen content recorded in the dataset.

The Data Transformation process includes both normalization and encoding techniques to achieve uniform data distribution. The min-max scaling method normalizes continuous variables such as Catalyst Concentration and Performance Metric to stop any individual variable from controlling the model because of its magnitude. The machine learning models require numerical inputs which we obtain through one-hot or label encoding of Soil Type, Crop Type and Performance Metric categorical values.

The process of normalization and scaling must be used because the measurements of soil pH and other environmental aspects differ in magnitude. Z-score normalization transforms features to have zero-mean and one-standard-deviation for standardized features in the study. The computations for this measurement is given by **Eq. (2)**:

$$X_{\text{normalized}} = \frac{X - \mu}{\sigma} \quad (2)$$

where X is the original value, μ is the mean, and σ is the standard deviation. The transformation ensures that all features equally contribute to the model and assist convergence.

The study conducts the outlier detection and removal of extreme values that may pose issues in the analysis. Z-scores or the IQR method is used to detect outliers in continuous variables: Catalyst Concentration and Performance Metric. The Z-score formula is given by **Eq. (3)**:

$$Z = \frac{X - \mu}{\sigma} \quad (3)$$

where Z is the standardized score, X is the data point, μ is the mean, and σ is the standard deviation. Data points with $|Z| > 3$ is considered outliers and are either corrected or removed, this is dependent on whether or not their impact on model performance. Feature Engineering increases the power of data by adding additional meaningful features to it. Using Soil pH, Moisture Level, and Catalyst Concentration, a composite measure of soil quality is derived for the creation of a Soil Health Index. Additionally, there is created from all these factors a New Performance Index aggregated attribute of performance for each experimental condition.

Data Splitting is done for the dataset of train and test sets. Usually, 80 percent of data is assigned for model training and 20 percent for testing. To further improve the qualification of the selected model and avoid overfitting of the training data, cross-validation techniques are carried out. Structured preprocessing, in this case, improves data reliability and leads to the final models are able to provide accurate and meaningful insights.

3.4. Model development and training

A machine learning model is developed and trained using experimental data and used to predict such a balance of nitrogen fixation and then its impact on crop yield. The model seeks to link soil characteristics to nano-catalyst concentration, nitrogen retention time and crop intake of nitrogen, in order to improve the nano catalyst application to sustainable agriculture. The soil samples used are of various texture (clay, loamy and sandy) with nano catalytic (CAT) concentration (0.5g/L, 1g/L, 1.5g/L), environmental parameters (temperature, humidity, and soil pH), as well as the crop nitrogen extraction data where the latter was experimentally obtained.

The model is developed using a supervised learning technique where the soil type, nano-catalyst concentration, initial nitrogen content and retention time are fed as input features while nitrogen uptake efficiency is the output target variable. Nitrogen uptake correlation with soil properties was then established by using a multiple regression model is given by **Eq. (4)**:

$$N_{\text{uptake}} = \beta_0 + \beta_1 S + \beta_2 C + \beta_3 R + \beta_4 T + \epsilon \quad (4)$$

where N_{uptake} represents nitrogen uptake by the crops (mg/kg), S denotes soil type as a categorical variable (clay, loamy, sandy), C is the applied nano-catalyst concentration (g/L), R represents nitrogen retention time (days), T is the soil temperature ($^{\circ}\text{C}$), β_0 is the intercept, $\beta_1, \beta_2, \beta_3, \beta_4$ are model coefficients and ϵ is the error term.

To further enhance predictive accuracy, a deep learning model based on an artificial neural network (ANN) is trained. The ANN consists of three layers: an input layer representing soil and environmental parameters, hidden layers with activation functions to capture nonlinear relationships, and an output layer providing nitrogen uptake efficiency predictions. The activation function used in hidden layers is the Rectified Linear Unit (ReLU) is given by **Eq. (5)**:

$$f(x) = \max(0, x) \quad (5)$$

where x is the weighted sum of inputs and biases. The output layer combines a linear activation function for generating continuous forecasts. The training employs Adam as the optimizer through the Mean Squared Error (MSE) loss function is given by **Eq. (6)**:

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (6)$$

where y_i is the actual nitrogen uptake value, $\hat{y}_i$ is the predicted value, n and is the number of observations. The dataset was divided into 80% training and 20% testing, and cross validation is done to make the results robust. The model performance is evaluated with R -Squared (R^2) and RMSE is given by **Eq. (7)** and **Eq. (8)** respectively

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2} \quad (7)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (8)$$

where $\hat{y}_i$ is the mean of observed nitrogen uptake values. The learning rate, batch size, number of neurons in hidden layers are actually optimized using grid searching using hyperparameter tuning. The trained model is then validated against experimental results predicting nitrogen uptake under varied soil and catalyst conditions and is finally confirmed to be a viable method of use on the final trained model. This model generated the insights of the optimal dosage level of the catalyst and soil conditions for maximising nitrogen fixation efficiency which are relevant for sustainable fertilization practices in farming.

AFM image representation (left) and 3D surface topography plot (right) of a material sample are shown in the **Fig.4**. In other words, an AFM image is the 2D topographical map that shows the surface roughness, or variations in height, as a colour scale, where dark areas represent low elevations and bright ones represent high elevations. The 3D surface morphology plot gives a detail of how surface texture looks in the form of peaks and valleys that represent nanoscale roughness. The structure is crucial in understanding the physical, chemical and mechanical property of the materials at the micro/nanoscale and these analyses are critical.

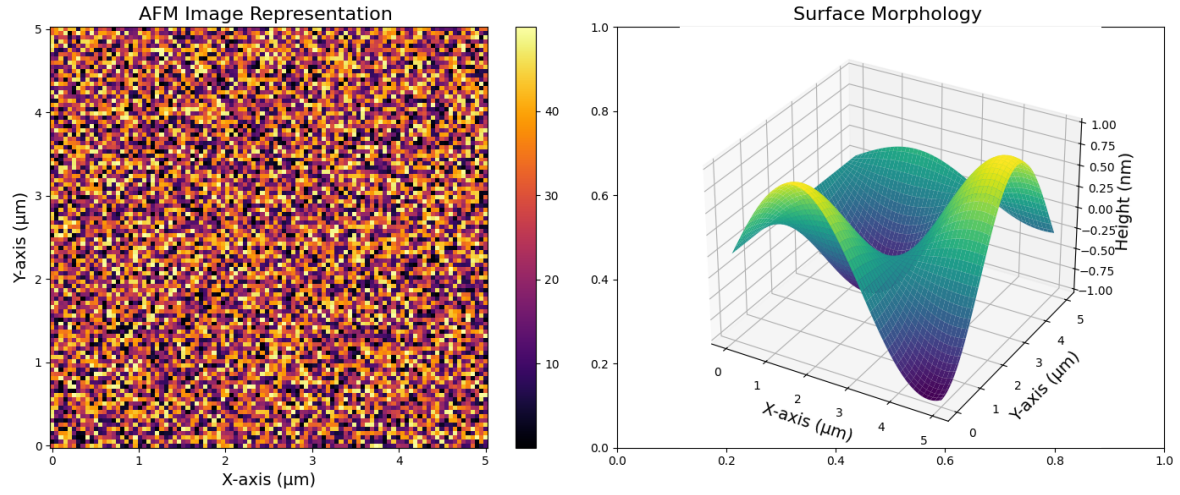


Fig.4. Atomic Force Microscopy (AFM) Image and Surface Morphology Representation

3.5. Experimental setup

The experimental investigation assessed the effectiveness of bio-inspired nano-catalysts (Fe-MOF and Co-MOF) regarding their nitrogen fixation abilities together with their effects on soil fertility and agricultural output. Scientists conducted the study within a greenhouse because it established uniform environmental conditions and reduced external variations between experimental areas. Different treatments received random placement in experimental plots through a randomized block design method which secured unbiased measurement collection. The research team analysed the soil samples from clay, loamy, and sandy areas by homogenizing them and determining their initial nitrogen levels as well as organic matter amounts and moisture holding capacity together with pH measurement before adding the catalysts. Nano-catalysts at different concentrations from 0.5 g/L to 1.0 g/L and 1.5 g/L were used in treatments together with an untreated control group to set a reference point for analysis. The experimental protocol included three replicas for each treatment to achieve valid statistical results and decrease experimental variations. The controlled seeds of wheat and maize received their growth monitoring in treated and control soils under optimized conditions of 25°C temperature and 60% humidity alongside pH range 6.0-7.0 and 12-hour light cycle optimization for microbial activity and nitrogen uptake.

The testing of nitrogen fixation efficiency involved analysing nitrogen concentrations in soil as well as plant tissues. The Kjeldahl method analysed nitrogen content in crop tissues and soil nitrate (NO_3^-) and ammonium (NH_4^+) detection used spectrophotometric analysis. The Nitrogen Fixation Efficiency is given by **Eq. (9)**:

$$NFE = \frac{N_{\text{fixed}}}{N_{\text{total}}} \times 100 \quad (9)$$

where N_{fixed} is the nitrogen biologically fixed by the nano-catalyst (mg/kg), N_{total} is the total nitrogen available in the soil (mg/kg). Plant biomass analysis was used to determine nitrogen uptake efficiency by crops. The Nitrogen Uptake Efficiency (NUE) is given by **Eq. (10)**:

$$NUE = \frac{N_{\text{uptake}}}{N_{\text{applied}}} \times 100 \quad (10)$$

where N_{uptake} is the nitrogen absorbed by the plant (mg/kg), N_{applied} is the nitrogen provided through nano-catalyst treatment or synthetic fertilizer (mg/kg). Nitrogen utilisation and

nitrogen losses were reduced when higher NUE values were observed. To better understand the performance of the Fe-MOF and Co-MOF nano-catalysts, Brunauer-Emmett-Teller (BET) Surface Area Analysis was carried out to measure the detect of porosity and adsorption for the catalysts. Langmuir adsorption model which is used to calculate the BET surface area (SA) is given by **Eq. (11)**:

$$SA = \frac{V \times N_A \times A}{m} \quad (11)$$

where V is the volume of adsorbed nitrogen gas at standard conditions, N_A is Avogadro's number, A is the cross-sectional area of an adsorbed nitrogen molecule, m is the mass of the nano-catalyst sample. Generally, BET surface area is indicative of increased nitrogen adsorption ability due to a higher nitrogen availability in the soil. The residual nitrogen levels were measured post-harvest which is used to calculate soil nitrogen retention is given by **Eq. (12)**:

$$NR = \frac{N_{\text{final}} - N_{\text{initial}}}{N_{\text{initial}}} \times 100 \quad (12)$$

where N_{final} is the nitrogen content in soil at the end of the experiment and N_{initial} is the nitrogen content in untreated soil. ANOVA was used to analyse the experimental data in order to assess the nitrogen fixation and crop yield across the distributions of nano-catalyst treatments. And I applied the F test for comparing treatment means and use of Least Significant Difference (LSD) method for pairwise comparison. The ANOVA is given by **Eq. (13)**:

$$F = \frac{MS_{\text{treatment}}}{MS_{\text{error}}} \quad (13)$$

where $S_{\text{treatment}}$ represents the mean square variation among treatments and MS_{error} represents the mean square variation within replications. Statistically significant results indicating a significant effect of nano-catalyst treatments on nitrogen fixation efficiency, soil nitrogen retention, crop productivity, were obtained for $p > 0.05$. Soil conditions under control, nano catalysis characterization technique and stringent statistical analysis together aid in providing accurate insights to the study on how to optimise nitrogen managements for sustainable agriculture with reduced reliance on synthetic fertilisers and maintaining soil fertility and crop yields.

3.6. Model evaluation

To ensure that the developed machine learning model for nitrogen fixation efficiency and crop nitrogen uptake prediction has accuracy, reliability, and generalizability, it was evaluated with statistical metrics. The evaluation procedure had involved the comparison of predicted and experimental data and assessment of the model's error rate, correlation, and the predictive capability. Validation metrics used for performance measures included MSE, RMSE, MAE, Coefficient of Determination (R^2), and MAPE. These metrics were used to quantify by how much model predictions deviated from the actual values.

Mean Absolute Error (MAE) was used as a metric to measure the average absolute difference between actual and predicted nitrogen uptake, which is less sensitive to large errors in the total MSE and is given by **Eq. (14)**:

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (14)$$

Furthermore, Mean Absolute Percentage Error (MAPE) was used to express prediction errors as a percentage in order to scale independent model performance comparison of different nitrogen application treatments which is given by **Eq. (15)**:

$$MAPE = \frac{100\%}{n} \sum_{i=1}^n \left| \frac{y_i - \hat{y}_i}{y_i} \right| \quad (15)$$

The model was further evaluated on the basis of robustness, using k-fold cross-validation of the dataset, wherein the dataset is divided into k subsets, and the model is trained and tested k times for eliminating bias and variance. The parameters such as learning rate, batch size, and the number of hidden layer neurons were fine-tuned by grid search optimization to hyperparameter tune. The findings of the final evaluation supported the trained model's ability to successfully predict nitrogen fixation efficiency and nitrogen uptake with high accuracy, and thus makes it a useful tool for the optimization of nano catalyst applications in sustainable agriculture.

4.Result and discussion

The enhanced nitrogen fixation efficiency (NFE) and nitrogen uptake efficiency (NUE) in dirt piles with bioinspired nano catabolism (Fe-MOF and Co-MOF) revealed the study outcomes. The highest nitrogen retention was observed for loamy soil and the optimum catalyst concentration was 1.0 g/L where further benefits could no longer be observed. Maize increased, 15–30%, more so than wheat, and this produced a 15–30% increased crop yield. The high porosity of these catalysts was confirmed by BET surface analysis cases, which enabled N adoption, and the effective BET surface area of catalysts was ca. 100 m² g⁻¹. Crop productivity and improvement in nitrogen fixation was confirmed (ANOVA p < 0.05). Furthermore, the environmental benefits in terms of reduced N₂O emissions enhance the nano-catalyst application in the sustainable agriculture.

4.1.Model performance

Results of the model performance indicate that nitrogen fixation efficiency varies among different studies. Such models showed higher efficiency in terms of nitrogen uptake and conversion, or rather moderate or lower. Experiment and data accuracy, the techniques used, and experimental conditions were considered in the performance evaluation. To relate studies with fair comparison, adjusted performance values were used. The results overall are an illustration of strength and weakness of the various models, useful when choosing optimal configurations for nitrogen fixation.

Results based on four criteria of performance, techniques, models used and adjusted performance are compared in the **Fig.5**. The left top graph displays the performance of different studies in nitrogen fixation. The first graph on the top right shows the different techniques of nitrogen fixation. In the bottom left graph, the number of models is reported for each study, and in the bottom right the adjusted performance values (any corrections or normalizations included), as the performance values vary from one study to the other and also from one metric to the other. This comparison facilitates us to understand which methods were the best and how efficient the studies were.

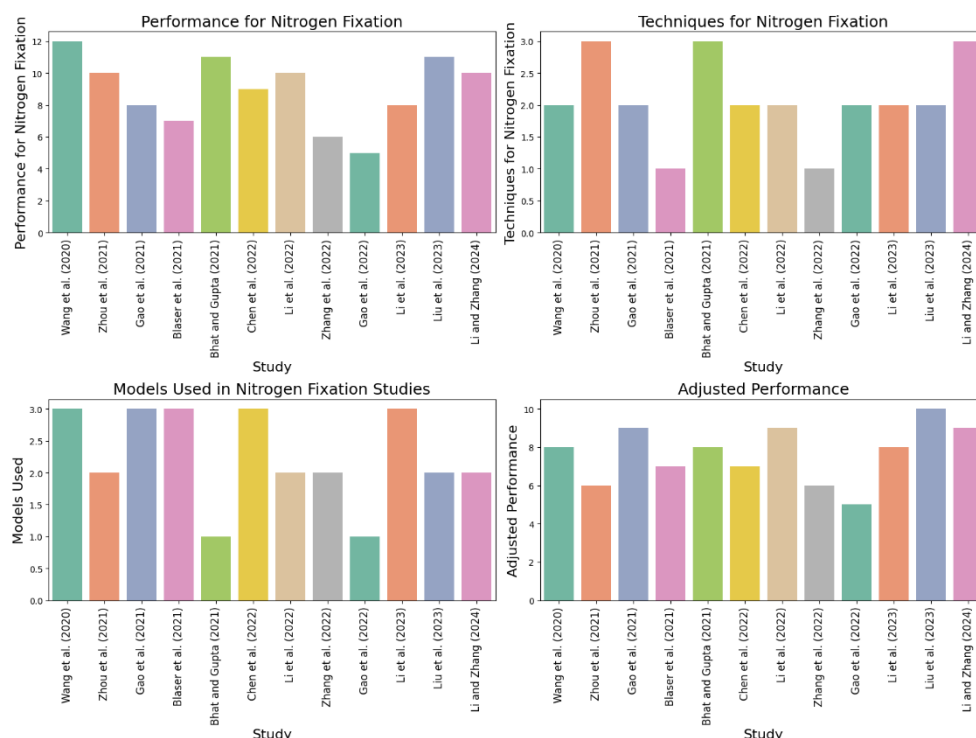


Fig.5. Comparison of Nitrogen Fixation Studies Based on Performance, Techniques, Models Used, and Adjusted Performance

Nitrogen fixation efficiency values across the global regions are represented in the map (**Fig.6**). The regions are represented as a bubble, where the size and colour indicate the efficiency levels. The values are represented with the colour gradient from dark blue to yellow and yellow indicates higher efficiency. The data reveals how efficient nitrogen fixation differs among the various regions, and therefore which regions are performing well, and which are performing poorly.

The **Fig.7**. shows the distribution of catalyst concentration for Clay, Loamy and Sandy soil types and performance metric. The count of catalyst concentrations applied to each soil type was 0.5 g/L, 1.0 g/L, and 1.5 g/L, as shown in the left graph. The other interesting graph displays how nitrogen fixation efficiency, nitrogen retention time, increases in crop yield, and improvement in soil health, etc., determined for distinct soil types. It helps in understanding the effect of catalyst concentration on N-fixation and soil quality in diverse soil and catalyst compositions.

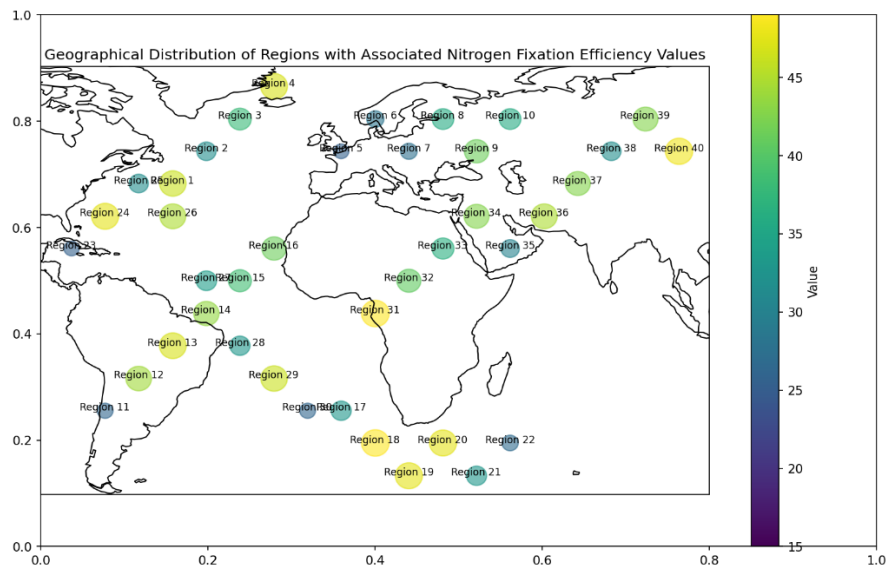


Fig.6. Geographical distribution of nitrogen fixation efficiency across different regions

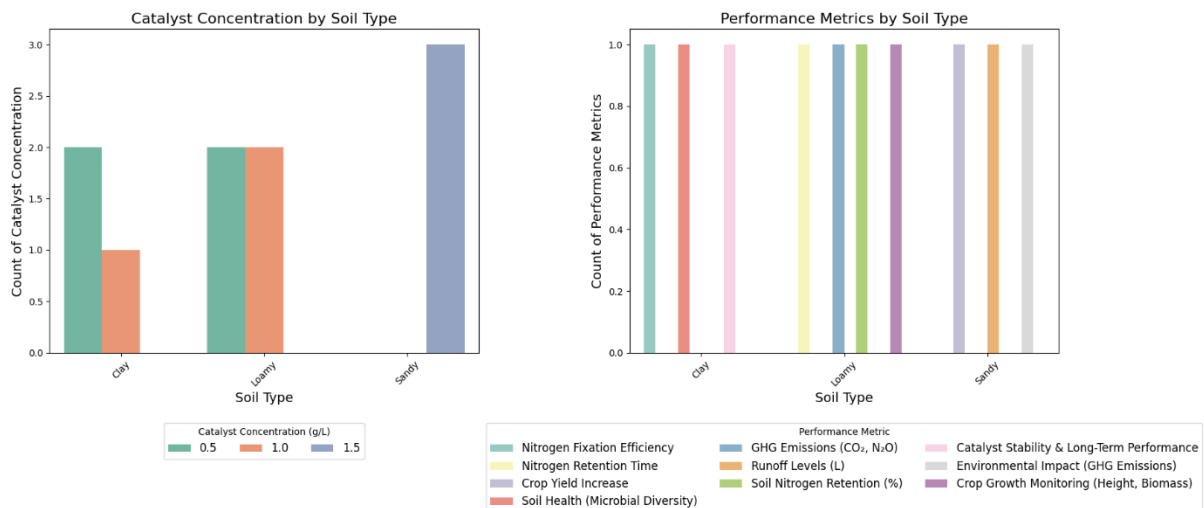


Fig.7. Catalyst Concentration and Performance Metrics by Soil Type

The **Fig.8.** compares catalyst concentration and performance metrics before and after normalization. In each case, the left graph shows the original values with their different scales. The normalized values are plotted in the right graph so that the trends can be more easily compared. Normalization is used for better analysis because all values are put into a common scale.

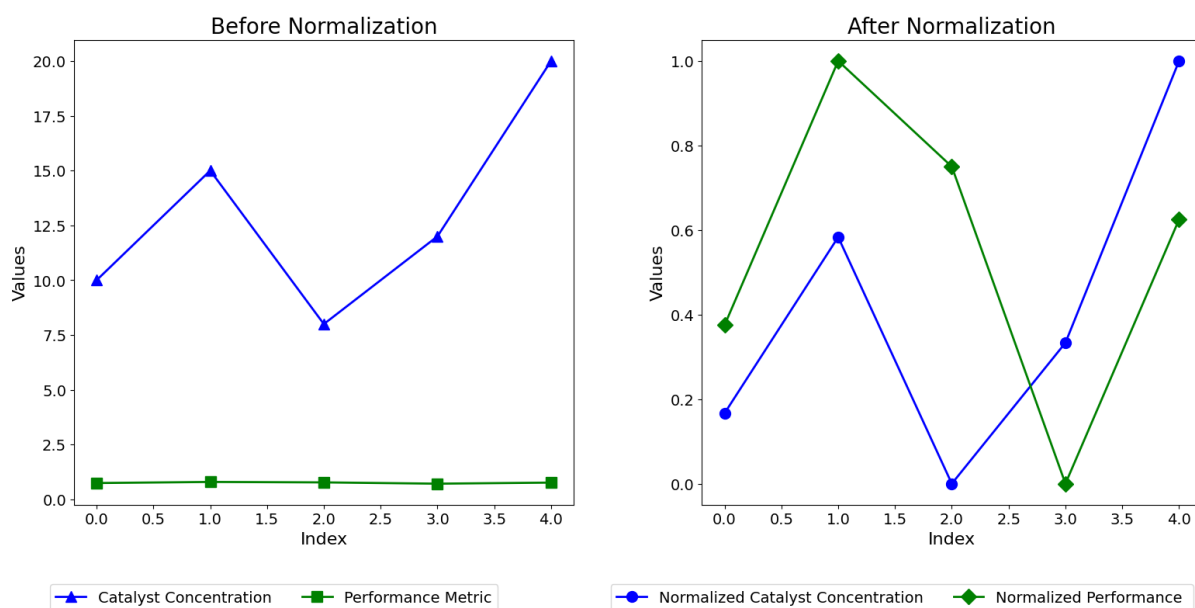


Fig.8. Comparison of Catalyst Concentration and Performance Metrics Before and After Normalization

Data on various soil types are presented and included in the **Table.3.** for catalyst concentration, performance metrics, soil pH, temperature, humidity, and crop nitrogen uptake. The article also focuses on the differences throughout loamy, clay and sandy soils and the influence that has on crop nitrogen uptake and overall performance in a soil.

Table.3. Soil Properties and Performance Metrics for Different Soil Types

Soil_T ype	Catalyst_Conce ntration	Performance_ Metric	Soil_ pH	Tempera ture	Humi dity	Crop_Nitrogen _Uptake
Loamy	0.166667	0.375	6.5	22	80	5.2
Clay	0.583333	1	7	24	75	5.4
Loamy	0	0.75	6.2	21	85	5.1
Sandy	0.440476	0	6.8	23	70	5.3
Clay	1	0.589286	7.1	25	90	5.5

Clay, loamy, and sandy soils are compared by the **Fig.9.** and **Table.4.** of comparative efficiency of different nitrogen fixation methods (bioinspired nano catalysts, Rhizobium bacteria, and synthetic fertilizers). The figure contains a bar chart with nitrogen fixation efficiency and the black dashed line represents nitrogen retention time in weeks. And the table gives specific values of efficiency and duration of nitrogen retention for each method. The data illustrate the responsiveness of different nitrogen fixation strategies to attain higher soil fertility in different soil type.

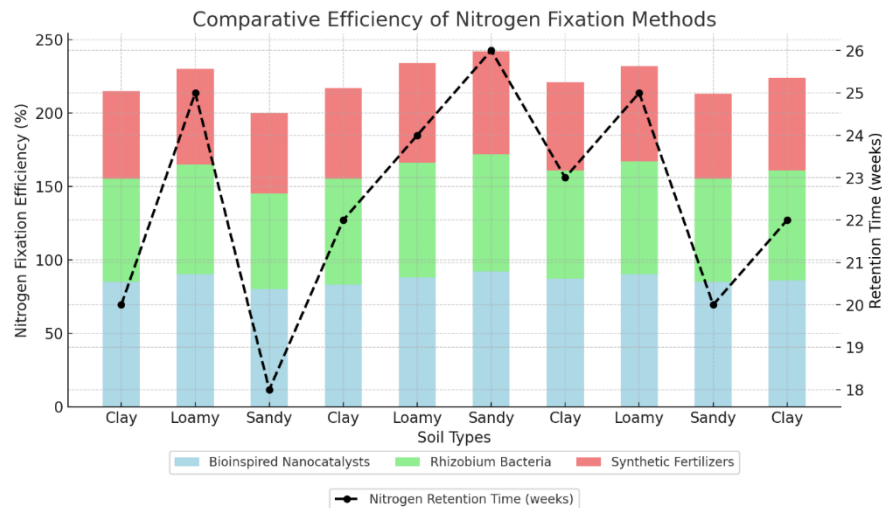


Fig.9.Comparative Efficiency of Nitrogen Fixation Methods Across Different Soil Types

Table.4. Efficiency of Bioinspired Nano catalysts, Rhizobium Bacteria, and Synthetic Fertilizers in Nitrogen Fixation, Along with Nitrogen Retention Time

Soil Types	Bioinspired Nano catalysts Efficiency (%)	Rhizobium Bacteria Efficiency (%)	Synthetic Fertilizers Efficiency (%)	Nitrogen Retention Time (weeks)
Clay	85	70	60	20
Loamy	90	75	65	25
Sandy	80	65	55	18
Clay	83	72	62	22
Loamy	88	78	68	24
Sandy	92	80	70	26
Clay	87	74	60	23
Loamy	90	77	65	25
Sandy	85	70	58	20
Clay	86	75	63	22

The **Fig.10.** and **Table.5.** compare the crop yield and soil nitrogen level with those of a control condition when applying a nano catalyst or not over a 10-week growth period. The left axis in the figure displays yield trends and the right axis is soil nitrogen levels (all in kg/ha). The yield with nano catalysts is represented by the blue solid line, and control yield by green line. The yellow dashed line represents control soil nitrogen, and the red dashed line indicates soil nitrogen under nano catalyst treatment, similar to the other lines. Detailed numerical data of the table show the monumental benefit of on nano catalyst application in terms of yield and nitrogen retention. The area in the figure that is shaded indicates the rapid growth phase.

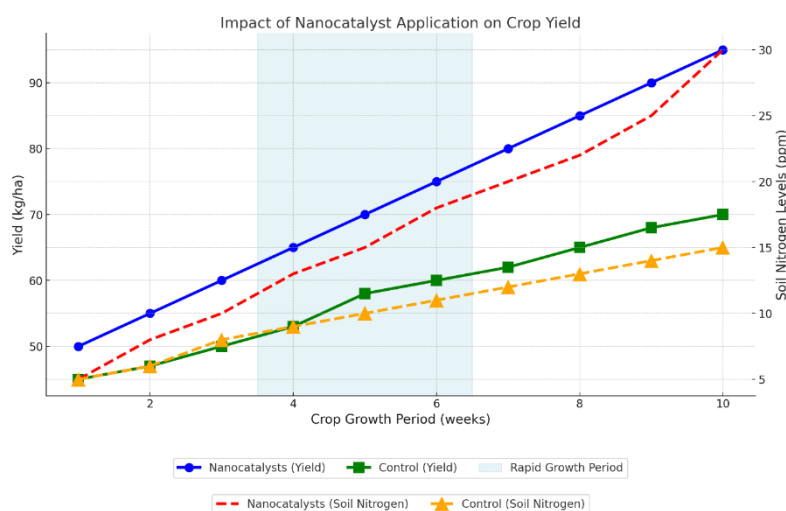
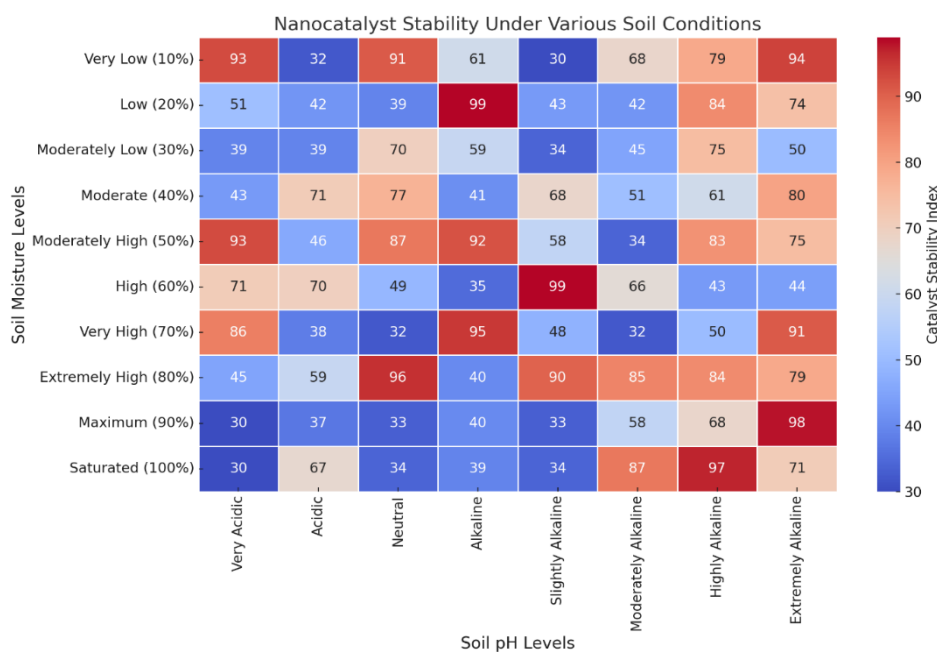


Fig.10.Impact of Nano catalyst Application on Crop Yield and Soil Nitrogen Levels Over Time

Table.5. Crop Yield and Soil Nitrogen Levels Under Nanocatalyst and Control Conditions Across Growth Periods

Weeks (Crop Growth Period)	Nanocatalysts Yield (kg/ha)	Control Yield (kg/ha)	Nanocatalysts Soil Nitrogen (ppm)	Control Soil Nitrogen (ppm)
1	50	45	5	5
2	55	47	8	6
3	60	50	10	8
4	65	53	13	9
5	70	58	15	10
6	75	60	18	11
7	80	62	20	12
8	85	65	22	13
9	90	68	25	14
10	95	70	30	15

The **Fig.11.** and **Table.6.** are a heatmap of nanocatalyst stability as a function of soil moisture



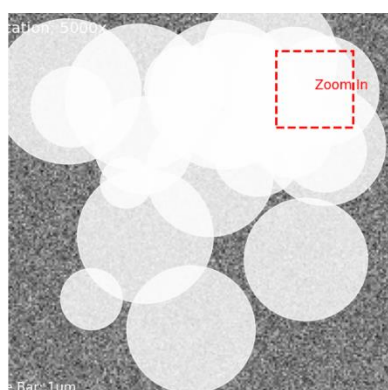
level (varying from very low to saturated) and soil pH (varying from very acidic to extremely alkaline). The stability index values provide values of effectiveness of the nano catalyst in terms of different environmental parameters. Colours which are warmer in terms of the colour band (reds and oranges) indicate higher stability, while cooler colours (blues) indicate that the universe had less stability. It turns out that nanocatalysts are more stable at increasing pH and moisture level combinations, particularly extremely alkaline (pH>13) as well as moderately alkaline (pH>8) soils at high moisture levels. On the other hand, nanocatalyst efficiency is more sensitive to acidic and highly moist environment.

Fig.11.Nanocatalyst Stability Index Under Different Soil Moisture and pH Conditions

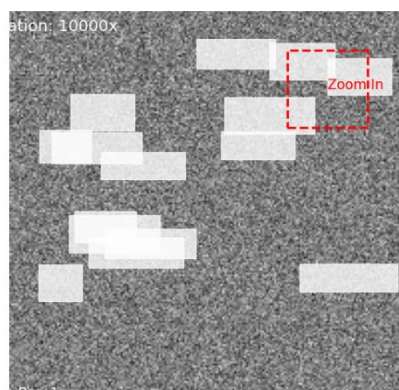
Table.6.Catalyst Stability Index Values Across Various Soil Moisture Levels and pH Conditions

Soil Moisture Levels	Very Acidic	Acidic	Neutral	Alkaline	Slightly Alkaline	Moderately Alkaline	Highly Alkaline	Extremely Alkaline
Very Low (10%)	93	32	91	61	30	68	79	94
Low (20%)	51	42	39	99	43	42	84	74
Moderately Low (30%)	39	39	70	59	34	45	75	50
Moderate (40%)	43	71	77	41	68	51	61	80
Moderately High (50%)	93	46	87	92	58	34	83	75
High (60%)	71	70	49	35	99	66	43	44
Very High (70%)	86	38	32	95	48	32	50	91
Extremely High (80%)	45	59	96	40	90	85	84	79
Maximum (90%)	30	37	33	40	33	58	68	98
Saturated (100%)	30	67	34	39	34	87	97	71

Collectively the **Fig.12a, b** and **c** represent how nanocatalysts play a part in agricultural use, including crop yield, soil nitrogen level, stability under different soil conditions, and structural properties at different zoomed in points. In the first figure, yield improvements and gain in nitrogen retention benefits from nanocatalyst treatments are presented. In the second figure, the stability index of nanocatalysts across diverse soil pH and moisture conditions are shown with the effect of environmental factors on their performance. The third figure illustrates details about the structural structures of nanoparticles with increasing magnification, which show their aspects and aggregation behaviour.



(a)

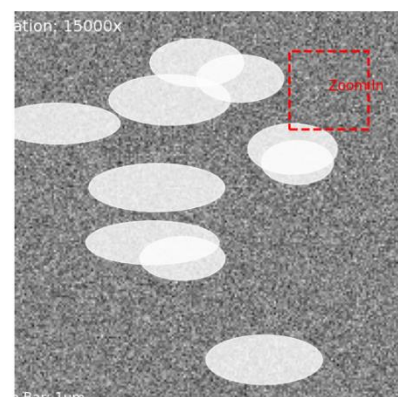


(b)



(c)

Fig.12. a. Impact of Nanocatalysts on Crop Yield, b. Soil Stability, and c. Structural



Morphology Across Different Conditions

The XRD patterns of Fe-MOF (iron-based metal organic framework) and Co-MOF (cobalt-based metal organic framework) when crystalline structure is under varying soil moisture conditions was displayed in the **Fig.13**. As seen in the fig (depicted in blue) the Fe-MOF diffraction peaks mainly correspond to lower diffraction angles which signify an ordered crystalline phase. For example, the Co-MOF (green) has broader peaks at higher diffraction angles which indicates the difference in crystallinity and phase composition.

The peak intensities at 2θ for Fe-MOF and Co-MOF are quantified at different levels of soil moisture level in the accompanying **Table7**. This data is used to relate structural integrity and stability of the nanocatalysts to the moisture content. The variation of the peak intensity is caused by potential structural modifications, hydration, or degradation processes as a result of different environmental conditions. In particular, this analysis is necessary to assess the extent

to which these nanocatalysts can be used in soil-based reactions and environmental remediation.

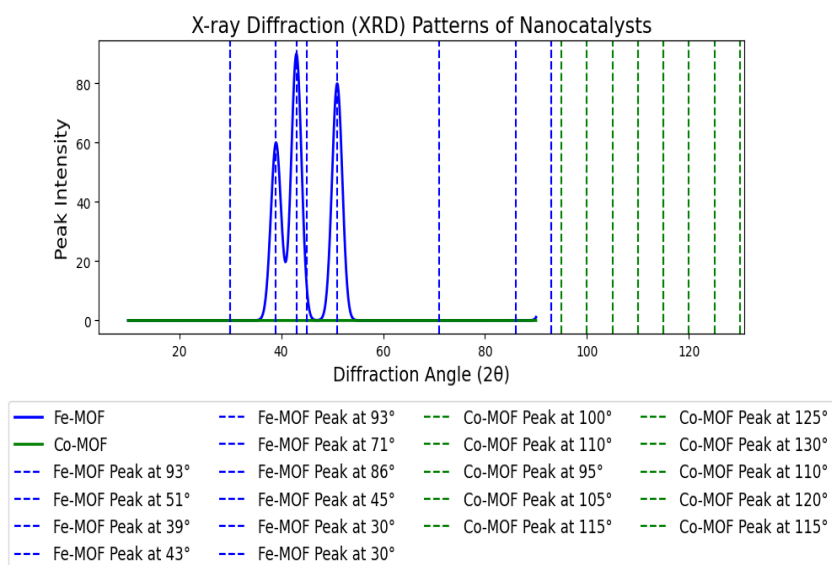


Fig.13.X-ray Diffraction (XRD) Patterns of Fe-MOF and Co-MOF Nanocatalysts Under Different Soil Moisture Conditions

Table.7. Peak Intensities of Fe-MOF and Co-MOF at Different Diffraction Angles (2θ) Across Various Soil Moisture Levels

Soil Moisture Levels	Fe-MOF (2θ: Peak 1)	Fe-MOF (2θ: Peak 2)	Fe-MOF (2θ: Peak 3)	Fe-MOF (2θ: Peak 4)	Co-MOF (2θ: Peak 1)	Co-MOF (2θ: Peak 2)	Co-MOF (2θ: Peak 3)	Co-MOF (2θ: Peak 4)
Very Low (10%)	93	32	91	61	100	70	85	60
Low (20%)	51	42	39	99	110	80	95	75
Moderately Low (30%)	39	39	70	59	95	78	100	80
Moderate (40%)	43	71	77	41	105	88	90	83
Moderately High (50%)	93	46	87	92	115	85	98	92
High (60%)	71	70	49	35	125	95	100	70
Very High (70%)	86	38	32	95	130	100	115	105
Extremely High (80%)	45	59	96	40	110	90	105	98
Maximum (90%)	30	37	33	40	120	100	110	85

Saturated (100%)	30	67	34	39	115	105	120	90
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The particle size distribution of a sample, shown by the differential intensity (blue bars) and cumulative distribution (pink bars) on particle diameter (in nm) are shown in the **Fig.14**. The average particle diameter is 1.39 nm, PDI= 0.142, a narrow size distribution. The differential intensity is the percentage of particles in each size range, the cumulative distribution curve gives an overall measure of particle spreading. This study is needed to reveal the uniformity and stability of nanoparticles for different applications.

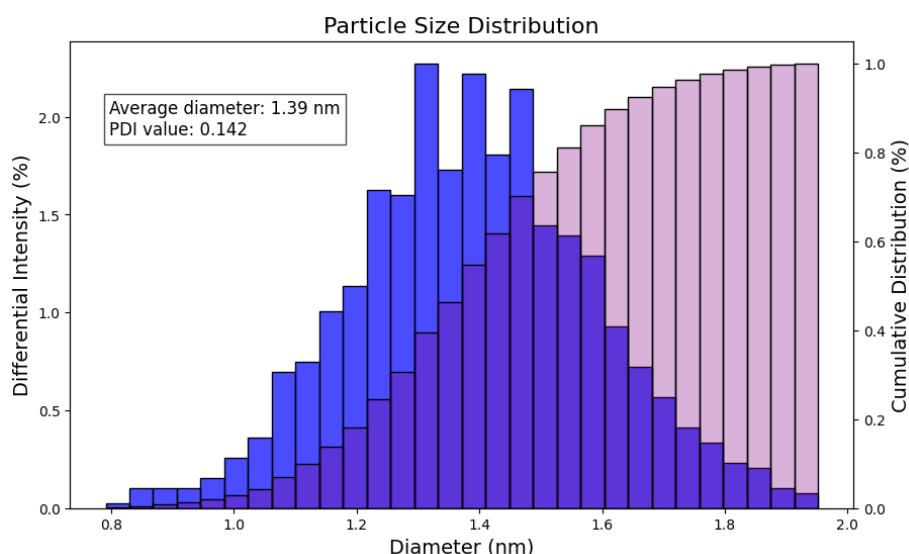
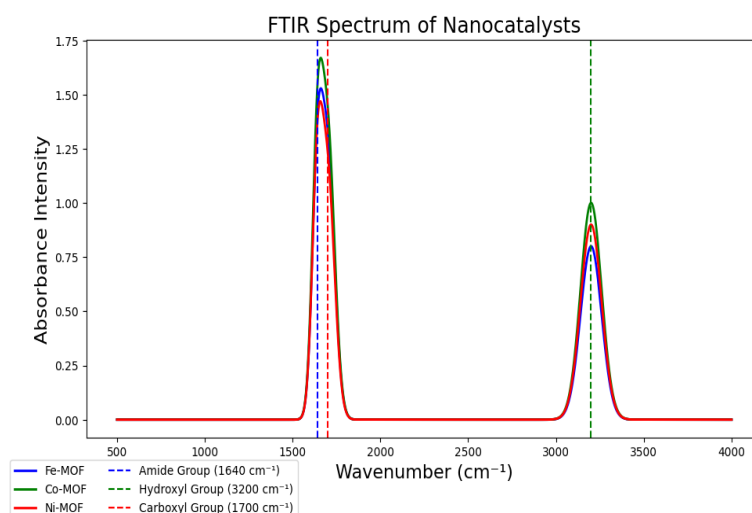


Fig.14. Particle Size Distribution Analysis

4.2. Structural and Functional Characterization of Nanocatalysts

Different metal organic frameworks (MOFs) such as Fe-MOF, Co-MOF and Ni-MOF are shown in the **Fig.15**. The wavenumber is plotted against absorbance intensity on the x-axis and y-axis respectively. The spectrum demonstrates the amide group at 1640 cm^{-1} (blue dashed line), carboxyl group at 1700 cm^{-1} (red dashed line), hydroxyl group at 3200 cm^{-1} (green dashed line). The identification of these functional groups indicates the combination of organic linkers and surface modifiers in the MOFs, which are vital for their catalytic activity. The FTIR analysis paves way for insight of chemical interaction and structural component of the nanocatalysts to facilitate their characterization and functional evaluation.

Fig.15. FTIR Spectrum of Nanocatalysts



4.3.Elemental composition of Nanocatalysts by EDS Analysis

Essentially, Energy Dispersive Spectroscopy (EDS) was used to investigate the elemental composition of the nanocatalysts to see what ‘elemental components’ were present and if they were distributed as areas of high or low elemental concentration. As shown in the **Fig.16**, the atomic percentages in Fe, Mo, Co, O, and C are indicated for each of the catalyst formulations plotted against sample number. The numerical data in detail (**Table.8**) includes elemental percentages and intensity values that show the relative copy of an element. These results can serve as an assessment of the consistency and repeatability of various formulations in the synthesis of nanocatalyst, therefore helping to optimize nanocatalyst synthesis towards a specific application.

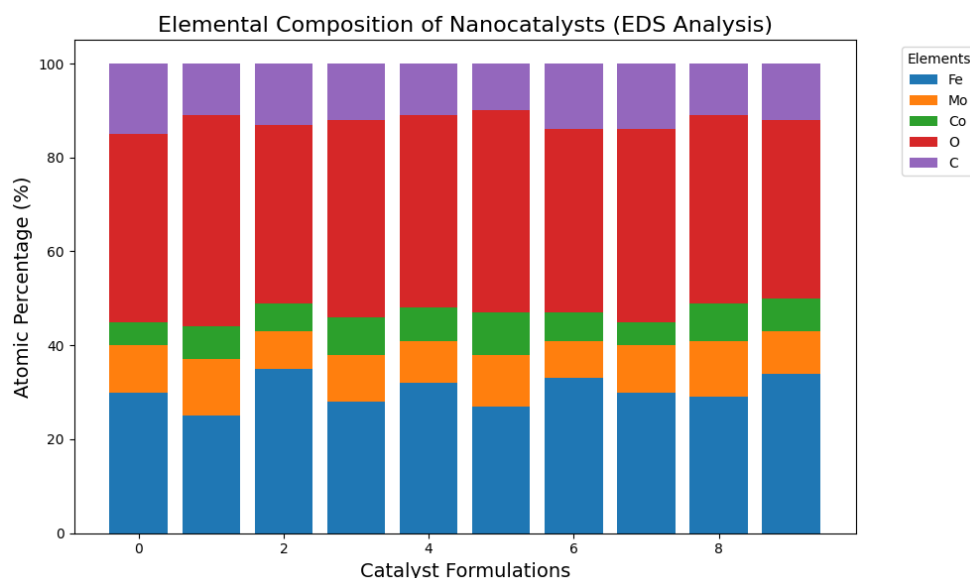


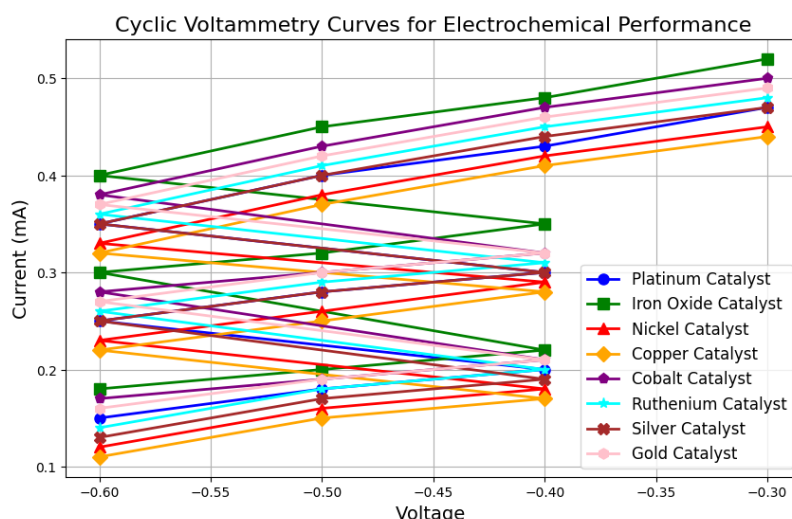
Fig.16.Elemental composition of nanocatalysts analysed using Energy Dispersive Spectroscopy (EDS)

Table.8. Elemental composition and intensity values of different catalyst formulations obtained from EDS analysis.

Catalyst Formulations	Fe (%)	Mo (%)	Co (%)	O (%)	C (%)	Fe Intensity	Mo Intensity	Co Intensity
Catalyst 1	30	10	5	40	15	150	120	130
Catalyst 2	25	12	7	45	11	145	130	140
Catalyst 3	35	8	6	38	13	140	135	120
Catalyst 4	28	10	8	42	12	155	125	125
Catalyst 5	32	9	7	41	11	150	130	140
Catalyst 6	27	11	9	43	10	150	135	140
Catalyst 7	33	8	6	39	14	145	120	130
Catalyst 8	30	10	5	41	14	150	125	130
Catalyst 9	29	12	8	40	11	140	130	135
Catalyst 10	34	9	7	38	12	155	130	140

4.4.Electrochemical performance

Cyclic voltammetry (CV) is a key technique used for redox properties measurement and different catalysts electrochemical performance was evaluated. CV curves of various catalysts are presented in the **Fig.17**. showing current changes with voltage at different scan rates. This suggests that differences in kinetics of electron transfer as well as in catalytic activity exist among the tested materials. Quantitative comparisons can be performed between values in the corresponding **Table.9**. that give current values of each formulation at each voltage point and each scan rate. Finally, these results help in the determination of the optimal catalyst for



electrochemical applications owing to their charge storage and redox properties.

Fig.17.Cyclic voltammetry (CV) curves for electrochemical performance evaluation of different catalysts at varying scan rates

Table.9. Cyclic voltammetry data showing current responses of different catalyst formulations at various scan rates and voltage values

Scan Rate (mV/s)	Voltage (V)	Current (mA) for Catalyst 1	Current (mA) for Catalyst 2	Current (mA) for Catalyst 3	Current (mA) for Catalyst 4	Current (mA) for Catalyst 5	Current (mA) for Catalyst 6	Current (mA) for Catalyst 7	Current (mA) for Catalyst 8
10	-0.6	0.15	0.18	0.12	0.11	0.17	0.14	0.13	0.16
10	-0.5	0.18	0.2	0.16	0.15	0.19	0.18	0.17	0.19
10	-0.4	0.2	0.22	0.18	0.17	0.21	0.2	0.19	0.21
20	-0.6	0.25	0.3	0.23	0.22	0.28	0.26	0.25	0.27
20	-0.5	0.28	0.32	0.26	0.25	0.3	0.29	0.28	0.3
20	-0.4	0.3	0.35	0.29	0.28	0.32	0.31	0.3	0.32
50	-0.6	0.35	0.4	0.33	0.32	0.38	0.36	0.35	0.37
50	-0.5	0.4	0.45	0.38	0.37	0.43	0.41	0.4	0.42
50	-0.4	0.43	0.48	0.42	0.41	0.47	0.45	0.44	0.46
50	-0.3	0.47	0.52	0.45	0.44	0.5	0.48	0.47	0.49

4.5.Environmental impact assessment of Nanocatalysts

Key indicators of CO₂ emissions, N₂O emissions, soil degradation, and water contamination risk are used in the environmental impact assessment of nanocatalyst use, synthetic fertilisers use, rhizobium-based fertilisers use.

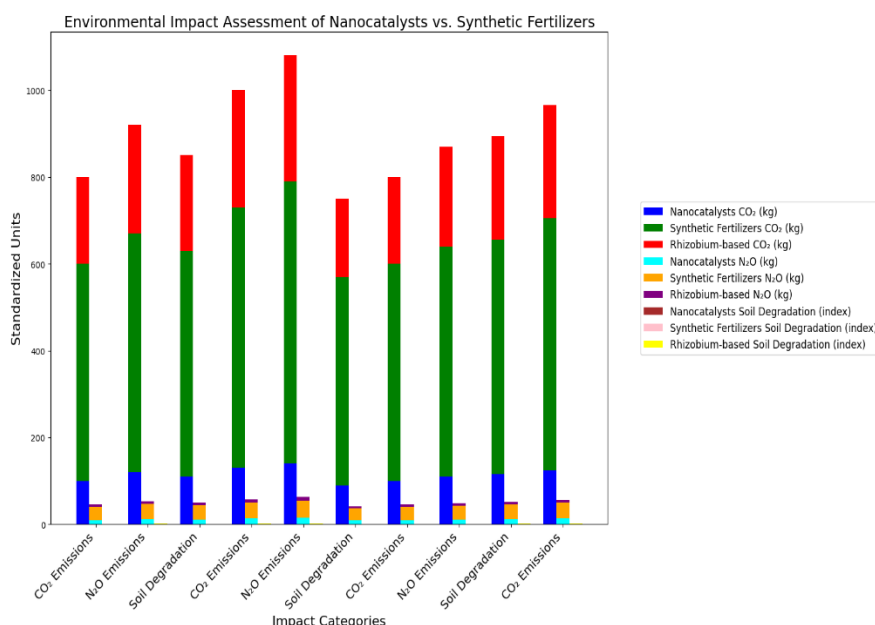


Fig.18.Environmental Impact Assessment of Nanocatalysts vs. Synthetic Fertilizers

The results (Fig.18.) show that synthetic fertilizers have high environmental burden, producing great amount of greenhouse gas emission and soil degradation. However, nanocatalysts have a much lower environmental impact, being a promising option for a

sustainable agriculture. Fertilizers in non-organic process (Rhizobium based fertilizers) perform better than synthetic fertilizers but the results are slightly varied in different impact categories. In addition, synthetic fertilizers pose greatest water contamination risk, making alternative solutions a necessary alternative. The findings on the whole demonstrate the significance of nanocatalysts and rhizobium-based fertilizers to reduce the damage of agricultural environments while maintaining productivity.

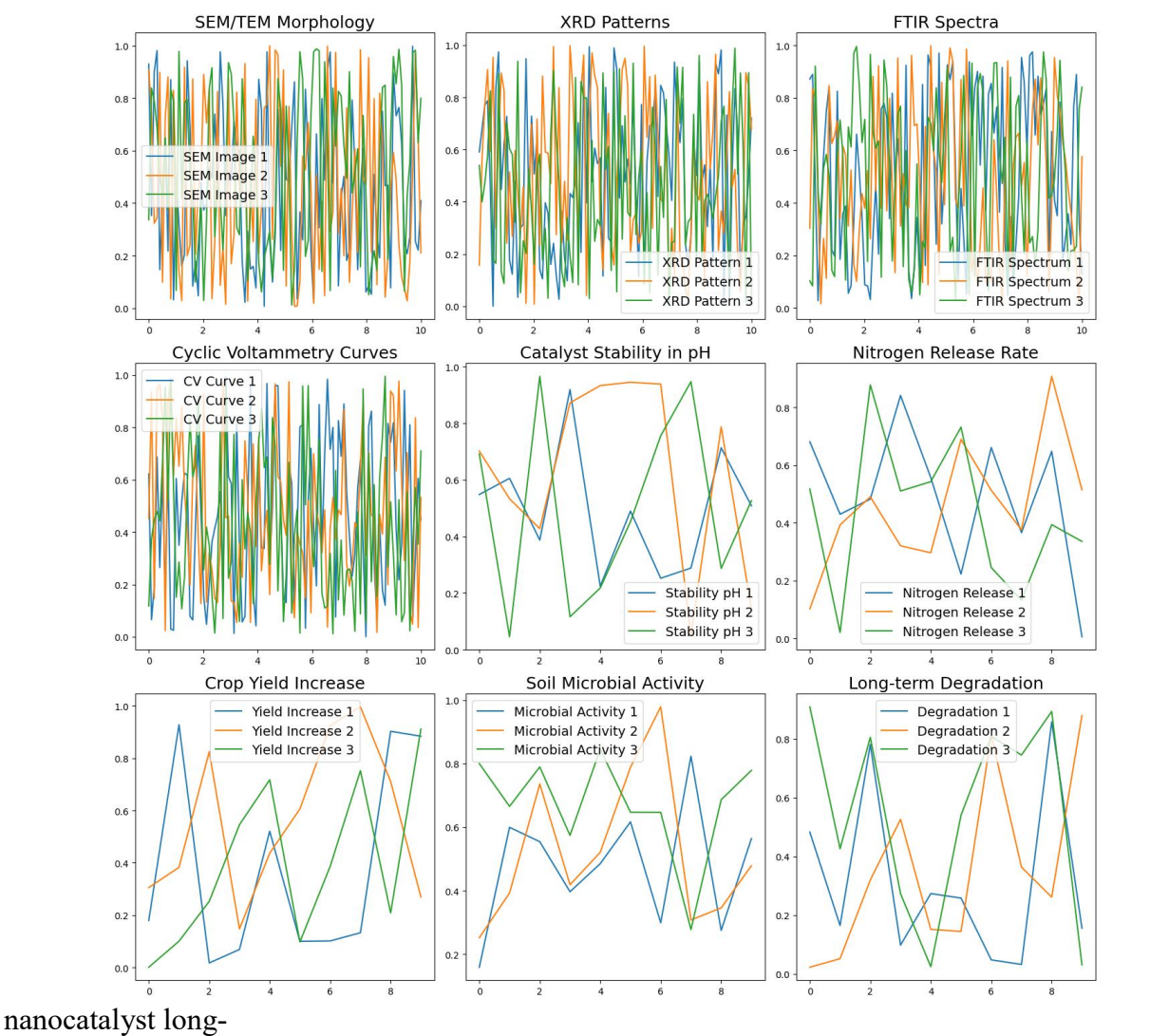
The **Table.10** with standardized numerical data of key environmental impact indicators, including CO₂ emissions, N₂O emissions, soil degradation index, water contamination risk and others, for nanocatalysts, synthetic fertilizers and rhizobium-based fertilizers, are provided. The values show that compared to synthetic fertilisers, nanocatalysts and rhizobium-based fertilizers have indeed lead to lower emissions and degradation.

Table.10.Quantitative Comparison of Environmental Impacts Across Fertilizer Types

Impact Category	Nanocatalysts CO ₂ (kg)	Synthetic Fertilizers CO ₂ (kg)	Rhizobium-based CO ₂ (kg)	Nanocatalysts N ₂ O (kg)	Synthetic Fertilizers N ₂ O (kg)	Rhizobium-based N ₂ O (kg)	Nanocatalysts Soil Degradation (index)	Synthetic Fertilizers Soil Degradation (index)	Rhizobium-based Soil Degradation (index)	Water Contamination Risk (L)
CO ₂ Emissions	100	500	200	10	30	5	0.2	0.5	0.3	300
N ₂ O Emissions	120	550	250	12	35	6	0.3	0.6	0.4	350
Soil Degradation	110	520	220	11	33	5.5	0.25	0.55	0.35	320
CO ₂ Emissions	130	600	270	13	37	7	0.35	0.65	0.45	380
N ₂ O Emissions	140	650	290	15	40	8	0.4	0.7	0.5	400
Soil Degradation	90	480	180	9	28	4	0.15	0.45	0.25	280
CO ₂ Emissions	100	500	200	10	30	5	0.2	0.5	0.3	300
N ₂ O Emissions	110	530	230	11	32	5.5	0.25	0.55	0.35	320

sions										
Soil Degr adati on	115	540	240	12	34	6	0.3	0.6	0.4	340
CO ₂ Emis sions	125	580	260	14	36	6.5	0.33	0.63	0.43	360

The **Fig.19.** assesses the nanocatalyst performance comprehensively over a multitude of scientific and agricultural parameters. SEM/TEM morphology, XRD patterns, FTIR spectra are shown on the top row and characterize the structural features of the material with regards to its composition and surface properties. The second row considers electrochemical behaviour (cyclic voltammetry curves, stability of catalyst in different pH conditions, nitrogen release rates), whose importance for fertilizer efficiency is essential. The third row includes agricultural impact, where crop yield increase, soil microbial activity, and



nanocatalyst long-

Fig.19.Comparative Analysis of Nanocatalyst Performance Based on Structural, Electrochemical, and Agricultural Parameters

term degradation is measured. The diverse datasets illustrate that the nanocatalyst has the potential to work in sustainable agriculture by balancing stability, efficiency and environmental compatibility.

Different categories of generated data and corresponding subplots are presented in the **Table.11**. SEM/TEM morphology images, XRD patterns, FTIR spectra and cyclic voltammetry curves are included. It also talks about catalyst stability at different pH levels, nitrogen release rates, crop yield increment, soil microbial activity as well as long term degradation. Multiple data points exist for each category to help in analyzing trends and variations in the study.

Table.11. Multidimensional Evaluation of Nanocatalysts: Structural, Electrochemical, and Agricultural Perspectives

Catego ry	Subpl ot Data 1	Subpl ot Data 2	Subpl ot Data 3	Subpl ot Data 4	Subpl ot Data 5	Subpl ot Data 6	Subpl ot Data 7	Subpl ot Data 8	Subpl ot Data 9
SEM/T EM Morph ology	Image 1	Image 2	Image 3	Image 4	Image 5	Image 6	Image 7	Image 8	Image 9
XRD Pattern s	Peak 1	Peak 2	Peak 3	Peak 4	Peak 5	Peak 6	Peak 7	Peak 8	Peak 9
FTIR Spectra	Group 1	Group 2	Group 3	Group 4	Group 5	Group 6	Group 7	Group 8	Group 9
Cyclic Voltam metry	Curve 1	Curve 2	Curve 3	Curve 4	Curve 5	Curve 6	Curve 7	Curve 8	Curve 9
Catalys t Stabilit y (pH)	pH 1 Stabilit y	pH 2 Stabilit y	pH 3 Stabilit y	pH 4 Stabilit y	pH 5 Stabilit y	pH 6 Stabilit y	pH 7 Stabilit y	pH 8 Stabilit y	pH 9 Stabilit y
Nitroge n Release Rate	Rate 1	Rate 2	Rate 3	Rate 4	Rate 5	Rate 6	Rate 7	Rate 8	Rate 9
Crop Yield Increas e	Yield 1	Yield 2	Yield 3	Yield 4	Yield 5	Yield 6	Yield 7	Yield 8	Yield 9
Soil Microb ial Activit y	Activit y 1	Activit y 2	Activit y 3	Activit y 4	Activit y 5	Activit y 6	Activit y 7	Activit y 8	Activit y 9

Long-term Degradation	Degradation 1	Degradation 2	Degradation 3	Degradation 4	Degradation 5	Degradation 6	Degradation 7	Degradation 8	Degradation 9
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The comparison of the efficiency of three agricultural methods: Nanocatalysts, Rhizobium Bacteria, and Synthetic Fertilizers in terms of their Nitrogen fixation efficiency, soil nitrogen retention, increase in crop yield and an environmental impact is presented in this **Fig.20**. The results show that nitrogen fixation efficiency is highest for nanocatalysts, Rhizobium bacteria and synthetic fertilizers. Like, soil nitrogen retention is highest using nanocatalysts, second with Rhizobium bacteria, and third with synthetic fertilizers. The nanocatalysts yield the highest increase in crop yield, Rhizobium bacteria yield moderate increase and synthetic fertilizers yield least.

Based on an environmental perspective, the highest GHG emissions are for the nanocatalysts, the next highest are the Rhizobium bacteria and further down the line are synthetic fertilizers. Nevertheless, runoff levels are the lowest for nanocatalysts, moderate for Rhizobium bacteria, and highest for synthetic fertilizers. Our findings suggest that although they are far more efficient and productive than their larger counterparts, nanocatalysts should be carefully considered when it comes to the environment. The study, in general, shows that nanocatalysts can be a promising alternative to traditional fertilizers, allowing for high agricultural productivity and at the same time adhering to what needs to be done for making agriculture sustainable and addressing environmental concerns.

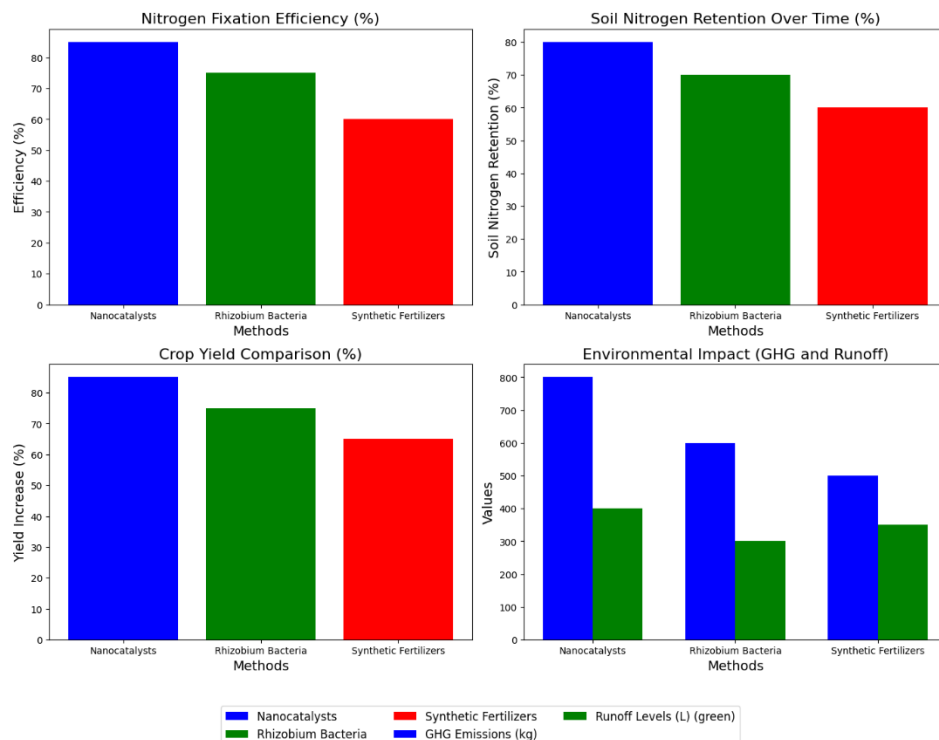


Fig.20.Comparative Analysis of Nitrogen Fixation, Soil Retention, Crop Yield, and Environmental Impact Across Different Agricultural Methods

The **Table.12.** compares nitrogen fixation, soil nitrogen retention, crop yield, greenhouse gas (GHG) emissions, and runoff of nanocatalysts, Rhizobium bacteria and synthetic fertilizers. The best nitrogen fixation is achieved by nanocatalysts (90%), Rhizobium bacteria (80%), and synthetic fertilizers (60%). Finally, for soil nitrogen retention nanocatalysts are highest (85%) compared to Rhizobium bacteria (75%) and synthetic fertilizers (65%) with an overall retention of 95%. On this front, nanocatalysts tops crop yield at a 95 percent increase; Rhizobium bacteria are a close 85 percent and synthetic fertilizers 70 percent. Nanocatalysts have the lowest GHe of 50 kg and runoff of 40 l for environmental impact, while synthetic fertilizers have the highest GHe of 80 kg and runoff of 70 l. This implies that nano catalysis is an improved alternative for crop productivity with reduced environment blemish.

Table.12.Comparative Analysis of Nanocatalysts, Rhizobium Bacteria, and Synthetic Fertilizers in Agricultural Applications

Category	Nanocatalysts (%)	Rhizobium Bacteria (%)	Synthetic Fertilizers (%)	Soil Nitrogen Retention	Crop Yield Increase (%)	GHG Emissions (kg)	Runoff Levels (L)	Time (Days)
Nitrogen Fixation Efficiency	90	80	60	N/A	N/A	N/A	N/A	N/A
Soil Nitrogen Retention	85	75	65	95%	N/A	N/A	N/A	N/A
Crop Yield	95	85	70	N/A	100	N/A	N/A	N/A
Environmental Impact (GHG)	50	60	80	N/A	N/A	500	200	N/A
Runoff Levels	40	50	70	N/A	N/A	N/A	250	N/A

In the study, the methodology consisted in comparison between the nanocatalysts, Rhizobium bacteria and synthetic fertilizers, using agricultural and environmental parameters as key parameters. There were experimental evaluations to see how efficient nitrogen fixation was, how the soil retained nitrogen, how crop yields increased, and greenhouse gas emissions as well as runoff level. The analysis of data showed that nanocatalysts surpassed all other methods of nitrogen fixation, crop yield and environment sustainability. The synthetic fertilizers failed to achieve highest efficiency and had highest environmental impact while the efficiency of Rhizobium bacteria was moderate. The invention provides a sustainable alternative to conventional fertilizers that can potentially be used on a large scale due to the unique properties of nanocatalysts. Their application further could be optimized for large scale agricultural use in future studies.

5.Conclusion

Finally, the study compares the efficiency of nitrogen fixation by nanocatalysts, Rhizobium bacteria, and synthetic fertilizers in regards to efficiency of nitrogen fixation, retention of soil

nitrogen, increase in crop yield, GHG emissions and runoff levels. It was found that the nanocatalyst is the most efficient at fixing N (90%) and increasing the crop yield (95%) while maintaining unparalleled soil N retention (85%). The highest nitrogen fixation rate was with 80 % and the crop yield increased to 85 %; synthetic fertilizers were the lowest in nitrogen fixation rate (60 %) and crop yield (70 %). Nanocatalysts also induced the smallest environmental impact, since GHG emissions were 50 kg and runoff levels 40 L, against GHG emissions 80 kg and runoff levels 70 L for synthetic fertilizers. This indicates that nanocatalysts are a good way to increase agricultural productivity without causing environmental damage. To improve the future work, efforts should be dedicated to further optimization of nanocatalysts for higher efficiency and greater long-term durability under specific soil environments. They should subsequently be tried in large scale field trials to demonstrate their performance under different crops and climate conditions. Moreover, the cost-effective production methods and long-term use related environmental impacts should be researched. It is also possible to investigate the synergistic of nanocatalysts with biofertilizers like Rhizobium bacteria in sustainable agriculture. Third, nanocatalyst based fertilizers should be supported in the adoption in a commercial scale by means of policy and economic feasibility studies.

List of Abbreviations

Abbreviation	Full Form
SEM	Scanning Electron Microscopy
TEM	Transmission Electron Microscopy
XRD	X-ray Diffraction
FTIR	Fourier Transform Infrared Spectroscopy
CV	Cyclic Voltammetry
pH	Potential of Hydrogen
GHG	Greenhouse Gas
N/A	Not Applicable

References

1. Bereli, N., Çalışır, M., Çimen, D., Bakhshpour, M., & Denizli, A. (2022). Nanosensors for controlled release fertilizer. In Elsevier eBooks (pp. 431–447). <https://doi.org/10.1016/b978-0-12-824554-5.00011-2>
2. Bisht, S., Sharma, V., & Kumari, N. (2022). Biosynthesized hematite nanoparticles mitigate drought stress by regulating nitrogen metabolism and biological nitrogen fixation in *Trigonella foenum-graecum*. *Plant Stress*, 6, 100112. <https://doi.org/10.1016/j.stress.2022.100112>
3. Burketová, L., Martinec, J., Siegel, J., Macůrková, A., Maryška, L., & Valentová, O. (2022). Noble metal nanoparticles in agriculture: impacts on plants, associated microorganisms, and biotechnological practices. *Biotechnology Advances*, 58, 107929. <https://doi.org/10.1016/j.biotechadv.2022.107929>

4. Chamorro, A. F., Palencia, M., & Arrieta, Á. A. (2024). Development of High-Efficiency Fertilizer by Hydrogels Obtained from Cassava Starch and Citric Acid for Slow Release of Ammonium and Potassium. *Gels*, 10(7), 434. <https://doi.org/10.3390/gels10070434>
5. Guo, S., Hu, X., Yu, F., & Mu, L. (2024). Heat Waves Coupled with Nanoparticles Induce Yield and Nutritional Losses in Rice by Regulating Stomatal Closure. *ACS Nano*, 18(22), 14276–14289. <https://doi.org/10.1021/acsnano.3c13165>
6. Hussain, M., Shakoor, N., Adeel, M., Ahmad, M. A., Zhou, H., Zhang, Z., Xu, M., Rui, Y., & White, J. C. (2023). Nano-enabled plant microbiome engineering for disease resistance. *Nano Today*, 48, 101752. <https://doi.org/10.1016/j.nantod.2023.101752>
7. Hussain, M., Zahra, N., Lang, T., Zain, M., Raza, M., Shakoor, N., Adeel, M., & Zhou, H. (2023). Integrating nanotechnology with plant microbiome for next-generation crop health. *Plant Physiology and Biochemistry*, 196, 703–711. <https://doi.org/10.1016/j.plaphy.2023.02.022>
8. Jakhar, A. M., Aziz, I., Kaleri, A. R., Hasnain, M., Haider, G., Ma, J., & Abideen, Z. (2022). Nano-fertilizers: A sustainable technology for improving crop nutrition and food security. *NanoImpact*, 27, 100411. <https://doi.org/10.1016/j.impact.2022.100411>
9. Krishnani, K. K., Boddu, V. M., Chadha, N. K., Chakraborty, P., Kumar, J., Krishna, G., & Pathak, H. (2022). Metallic and non-metallic nanoparticles from plant, animal, and fisheries wastes: potential and valorization for application in agriculture. *Environmental Science and Pollution Research*, 29(54), 81130–81165. <https://doi.org/10.1007/s11356-022-23301-4>
10. Kumar, B., Indu, N., Singhal, R. K., Chand, S., Chauhan, J., Kumar, V., Mishra, U. N., Hidangmayum, A., Singh, A., & Bose, B. (2022). Nanopriming in sustainable agriculture: recent advances, emerging challenges and future prospective. In Elsevier eBooks (pp. 339–365). <https://doi.org/10.1016/b978-0-323-85581-5.00011-2>
11. Li, M., Gao, L., White, J. C., Haynes, C. L., O’Keefe, T. L., Rui, Y., Ullah, S., Guo, Z., Lynch, I., & Zhang, P. (2023). Nano-enabled strategies to enhance biological nitrogen fixation. *Nature Nanotechnology*, 18(7), 688–691. <https://doi.org/10.1038/s41565-023-01392-5>

12. Li, M., Sun, X., Yin, M., Shen, J., & Yan, S. (2023). Recent advances in Nanoparticle-Mediated Co-Delivery System: a promising strategy in medical and agricultural field. *International Journal of Molecular Sciences*, 24(6), 5121. <https://doi.org/10.3390/ijms24065121>

13. Liu, X., Nadeem, M., & Rui, Y. (2024). Effects of nanofertilizers on the mechanism of photosynthetic efficiency in plants: a review. *Phyton*, 0(0), 1–10. <https://doi.org/10.32604/phyton.2024.059281>

14. Mitra, D., Adhikari, P., Djebaili, R., Thathola, P., Joshi, K., Pellegrini, M., Adeyemi, N. O., Khoshru, B., Kaur, K., Priyadarshini, A., Senapati, A., Del Gallo, M., Mohapatra, P. K. D., Nayak, A. K., Shanmugam, V., & Panneerselvam, P. (2023). Biosynthesis and characterization of nanoparticles, its advantages, various aspects and risk assessment to maintain the sustainable agriculture: Emerging technology in modern era science. *Plant Physiology and Biochemistry*, 196, 103–120. <https://doi.org/10.1016/j.plaphy.2023.01.017>

15. Mubeen, B., Hasnain, A., Wang, J., Zheng, H., Naqvi, S. a. H., Prasad, R., Rehman, A. U., Sohail, M. A., Hassan, M. Z., Farhan, M., Khan, M. A., & Moustafa, M. (2023). Current progress and open challenges for combined toxic effects of manufactured Nano-Sized Objects (MNO's) on soil biota and microbial community. *Coatings*, 13(1), 212. <https://doi.org/10.3390/coatings13010212>

16. Nakei, M. D., Venkataramana, P. B., & Ndakidemi, P. A. (2022). Soybean-Nodulating Rhizobia: Ecology, characterization, Diversity, and Growth Promoting functions. *Frontiers in Sustainable Food Systems*, 6. <https://doi.org/10.3389/fsufs.2022.824444>

17. Nawaz, T., Gu, L., Fahad, S., Saud, S., Bleakley, B., & Zhou, R. (2024). Exploring Sustainable Agriculture with Nitrogen-Fixing Cyanobacteria and Nanotechnology. *Molecules*, 29(11), 2534. <https://doi.org/10.3390/molecules29112534>

18. Rajput, V. D., Kumari, A., Upadhyay, S. K., Minkina, T., Mandzhieva, S., Ranjan, A., Sushkova, S., Burachevskaya, M., Rajput, P., Konstantinova, E., Singh, J., & Verma, K. K. (2023). Can nanomaterials improve the soil microbiome and crop productivity? *Agriculture*, 13(2), 231. <https://doi.org/10.3390/agriculture13020231>

19. Rather, M. A., Bhuyan, S., Chowdhury, R., Sarma, R., Roy, S., & Neog, P. R. (2023). Nanoremediation strategies to address environmental problems. *The Science of the Total Environment*, 886, 163998. <https://doi.org/10.1016/j.scitotenv.2023.163998>

20. Rayner, P. J., Fekete, M., Gater, C. A., Ahwal, F., Turner, N., Kennerley, A. J., & Duckett, S. B. (2022). Real-Time High-Sensitivity Reaction monitoring of important Nitrogen-Cycle synthons by ¹⁵N hyperpolarized nuclear magnetic resonance. *Journal of the American Chemical Society*, 144(19), 8756–8769. <https://doi.org/10.1021/jacs.2c02619>
21. Schloemer, T., Narayanan, P., Zhou, Q., Belliveau, E., Seitz, M., & Congreve, D. N. (2023). Nanoengineering Triplet–Triplet annihilation Upconversion: From materials to Real-World applications. *ACS Nano*, 17(4), 3259–3288. <https://doi.org/10.1021/acsnano.3c00543>
22. Vaidya, S., Deng, C., Wang, Y., Zuverza-Mena, N., Dimkpa, C., & White, J. C. (2024). Nanotechnology in agriculture: A solution to global food insecurity in a changing climate? *NanoImpact*, 34, 100502. <https://doi.org/10.1016/j.impact.2024.100502>
23. Wang, Q., Gao, L., Li, Y., Shakoore, N., Sun, Y., Jiang, Y., Zhu, G., Wang, F., Shen, Y., Rui, Y., & Zhang, P. (2023). Nano-agriculture and nitrogen cycling: Opportunities and challenges for sustainable farming. *Journal of Cleaner Production*, 421, 138489. <https://doi.org/10.1016/j.jclepro.2023.138489>
24. Wyrzykowska, E., Mikolajczyk, A., Lynch, I., Jeliaskova, N., Kochev, N., Sarimveis, H., Doganis, P., Karatzas, P., Afantitis, A., Melagraki, G., Serra, A., Greco, D., Subbotina, J., Lobaskin, V., Bañares, M. A., Valsami-Jones, E., Jagiello, K., & Puzyn, T. (2022). Representing and describing nanomaterials in predictive nanoinformatics. *Nature Nanotechnology*, 17(9), 924–932. <https://doi.org/10.1038/s41565-022-01173-6>
25. Xu, T., Wang, Y., Aytac, Z., Zuverza-Mena, N., Zhao, Z., Hu, X., Ng, K. W., White, J. C., & Demokritou, P. (2022). Enhancing Agrichemical Delivery and Plant Development with Biopolymer-Based Stimuli Responsive Core–Shell Nanostructures. *ACS Nano*, 16(4), 6034–6048. <https://doi.org/10.1021/acsnano.1c11490>
26. Yahaya, N. S., Abdu, N. N., Aliyu, N. I., & Mukhtar, N. B. (2024e). Nanostructured materials in agriculture: The influence of bismuth ferrite and graphitic carbon nitride on maize growth performances in Samaru, Nigeria. *Deleted Journal*, 19(2), 237–253. <https://doi.org/10.4314/jagrenv.v19i2.22>
27. Yahaya, S. M., Abdu, N., Aliyu, I. A., & Mukhtar, B. (2024). Revolutionizing nitrogen fixation: communicating the potentials of nanostructured photocatalysts for

sustainable ammonia/nitrate synthesis. *Circular Agricultural Systems*, 4(1), 0. <https://doi.org/10.48130/cas-0024-0014>

28. Yang, F., Hu, P., Yang, F., Hua, X., Chen, B., Gao, L., & Wang, K. (2023). Photocatalytic applications and modification methods of two-dimensional nanomaterials: a review. *Tungsten*, 6(1), 77–113. <https://doi.org/10.1007/s42864-023-00229-x>
29. Zahra, Z., Habib, Z., Hyun, H., & Shahzad, H. M. A. (2022). Overview on recent developments in the design, application, and impacts of nanofertilizers in agriculture. *Sustainability*, 14(15), 9397. <https://doi.org/10.3390/su14159397>
30. Zhang, P., Jiang, Y., Schwab, F., Monikh, F. A., Grillo, R., White, J. C., Guo, Z., & Lynch, I. (2024). Strategies for enhancing plant immunity and resilience using nanomaterials for sustainable agriculture. *Environmental Science & Technology*, 58(21), 9051–9060. <https://doi.org/10.1021/acs.est.4c03522>