VOL. 08 NO. 9,
MAY, 2025
E-ISSN 3026-958X
P-ISSN 3027-1169

African Scholar Publications & Research International
www.africanscholarpub.com

Journal of Science Innovation & Technology Research (JSITR)

Machine Learning in Nanoparticles Toxicology: Mechanisms, Predictive Modelling, and Risk Assessment Strategies

Ubong Bernard Essien[1]; Akaninyene U. Akpan[1]; Felix Isidore Ibanga[2]; Itu Prince-Charles Omin[3]; Prince Uche Micheal[4]; Bright Akachi Daniel[5]; and Linda I. Ozohili[6]

[1]Animal and Environmental Biology, Faculty of Science, University of Uyo, Akwa Ibom State. [2]Department of Sustainability and Environmental Management, Faculty of Engineering, Environment and Computing, Coventry University, United Kingdom. [3]Department of Environmental Resource Management, University of Calabar, Calabar. [4]Department of Pure and Industrial Chemistry, University of Port Harcourt. [5]Department of Chemistry, University of Tennessee, Knoxville. [6]Department of Microbiology, Faculty of Science, University of Port Harcourt

Correspondence author: ubongessien11@gmail.com
DOI: https://doi.org/10.70382/ajsitr.v8i9.043

Abstract

The increasing application of engineered nanoparticles (ENPs) in industry and medicine will require economic and ethically acceptable procedures for toxicological assessment. This paper employed supervised machine learning (ML) to model a new set of physicochemical data, correlating the 312 ENP samples contained in the eNano-Mapper database with ENP cytotoxicity. The major characteristics were particle size (mean = 68.5 nm), zeta potential (=18.6 mV), hydrodynamic diameter (102.3 nm), surface area, as well as solubility. Four approaches of ML: Logistic Regression (LR), Support Vector Machine (SVM), Random Forest (RF), and Extreme Gradient Boosting (XGBoost), have been tested, and XGBoost demonstrated 91% accuracy, 0.90 precision, 0.89 recall, 0.89 F1-score, and *Area Under the* Receiver Operating Characteristic *(ROC) Curve (*AUC) = 0.94. The Logistic Regression and SVM models reported lower scores (accuracy: 78% and 80%, AUC: 0.81 and 0.83, respectively),

indicating a diminished capacity to identify non-linear toxicological trends. The SHAP analysis provided zeta potential (0.146), hydrodynamic diameter (0.131), and particle size (0.112) as the best predictive factors of toxicity. Particle size showed a significant correlation with hydrodynamic diameter (r = 0.78), suggesting that future testing procedures could be redundant. There were only five entries (misclassifications), with the majority between the high and moderate toxicity categories. The research presents a compelling, fact-based alternative to animal testing, thereby driving the development of safer-by-design nanoparticles and enhancing risk assessment.

Keywords: Nanotoxicology, Explainable AI, Engineered Nanoparticles (ENPs), SHAP Analysis, Predictive Toxicity Modelling.

Introduction

The advent of nanotechnology has disrupted many industrial and biomedical sectors because it allows controlling the atomic and molecular level of materials. Engineered nanoparticles (ENPs), which are considered those with one dimension under 100 nanometres, are rapidly introduced into cosmetics, pharmaceutical products, food packaging, electronics, and agricultural products (Mishra *et al*., 2025; Gudainiyan *et al*., 2024). Nanoscale materials may exhibit pronounced and distinctive morphological and chemical behaviours, differing from their bulk-like counterparts in terms of higher chemical reactivity, greater mechanical strength, and enhanced biological activity. The peculiarities of these materials, however, raise questions about their interactions with the rest of the biological environment, which should be thoroughly evaluated from a toxicological perspective. Conventional toxicological testing of nanoparticles primarily relies on in vitro and in vivo testing to identify undesired effects, which include oxidative stress, DNA damage, inflammatory processes, and cellular apoptosis (Batir-Marin *et al*., 2025). Even though such approaches have provided significant benefits in terms of attaining mechanistic knowledge, they can be cumbersome in terms of resource consumption, are lengthy, and involve controversial aspects related to the use of animals in testing such developments. More importantly, the continuously growing types of nanoparticles with different compositions, sizes, shapes, surface charges, and functionalization orders prohibit extensive experimental testing. This necessitates the urgent need to provide alternative, efficient and scalable methods in predicting and interpreting nanoparticle toxic potentials. The latest developments in data science and artificial intelligence (AI) hold significant potential

for addressing life-altering problems in nanotoxicology. With high-quality datasets, machine learning (ML) algorithms can identify the existence of complex and nonlinear relationships between nanoparticle physicochemical properties and their biological effects (Islam *et al*., 2025). Such predictive models not only improve on the identification of hazards but also offer mechanistic reasoning using feature attribution methods, including Shapley Additive exPlanations (SHAP) and Local Interpretable Model-Agnostic Explanations (LIME). In addition, quantitative structure-activity relationships (QSAR), Risk Categorisation (RC), and nanoparticle library virtual screening are also leveraging the use of AI-based tools to a large extent. This research aims to contribute to this new paradigm by developing and testing AI-based models for nanoparticle toxicity predictions, utilising publicly accessible toxicological databases. In particular, the paper investigates how several supervised machine learning algorithms perform in predicting cytotoxicity endpoints, which physicochemical predictors are the most important determinants of nanoparticle behaviour, and what larger significance such models have for regulatory toxicology and environmental safety. By adopting this integrative approach, the manuscript aims to bridge that gap and lay the groundwork for developing smarter, faster, and more ethical risk assessment frameworks applicable in the era of nanotechnology.

Literature Review

With the increasing use of engineered nanoparticles (ENPs) in medicine, agriculture, and manufacturing, there has also been an increased interest in their potential toxicity. Researchers like Attallah *et al*. (2025), Desai *et al*. (2025), Teli *et al*. (2024), and Acharya *et al*. (2025) have, in distinct studies, reported that the physicochemical properties of nanoparticles, namely size, charge, shape and solubility, among others, significantly impact the biological behaviour and toxicological aspects of nanoparticles. However, this enormous variety in the forms and properties of nanoparticles has precluded the use of these massive toxicology tests using classical methods of in vivo and in vitro testing, which is not only unrealistic but also unethical. Artificial intelligence (AI) and machine learning (ML) are other technologies that are proving useful in the field of nanotoxicology, aiming to mitigate these drawbacks. Some of these studies have successfully implemented supervised learning models, such as random forest, support vector algorithm, and gradient boosting, to predict the endpoints of toxicity, including oxidative stress, genotoxicity, and cytotoxicity, using physicochemical descriptors. The repetition of observations from the work by Puzyn *et al*. (2011), Li *et al*. (2022) and Islam *et al*. (2025) were especially useful for highlighting the positive effects of QSAR modelling on nanoparticles, thereby establishing a connection between surface chemistry and toxicity results.

Current development efforts have focused on enhancing model interpretability through explainable AI approaches, such as SHAP and LIME, to identify the most significant nanoparticle features that contribute to a toxic response. In parallel, open-access databases,

including eNano Mapper and NanoHub, have supported data-driven modelling endeavours, although the disparity in quality and standardisation of data remains an issue. Although the developed AI models have achieved success, the majority of them are limited due to the heterogeneity of the dataset, lack of external validation, and regulatory acceptance. These demonstrate the relevance of stronger, more interpretable, and practically usable modelling frameworks at the intersection of data science and mechanistic toxicology, enabling effective risk assessment.

In this study, a refined dataset obtained from the eNano-Mapper database, featuring experimentally proven toxicological data and physicochemical properties of engineered nanoparticles (ENPs), was utilised. The database consisted of a variety of metal nanoparticles (for instance, silver, titanium dioxide, zinc oxide) and their related properties, including size, zeta potential, hydrodynamic diameter, surface area, solubility, and shape. The primary endpoints evaluated in the toxicity assessment were cell viability (IC50 values) and markers of oxidative stress, as determined by in vitro experiments. Data preprocessing consisted of data cleaning, replacement of missing values using imputation methods, normalisation by Min-Max values on numerical features, and assigning labels to categorical features. Correlation analysis and Recursive Feature Elimination were used to select the most predictive variables. To classify nanoparticle toxicity into low, moderate or high, four supervised machine learning models were constructed: Logistic Regression, Random Forest, Support Vector Machine (SVM), and Extreme Gradient Boosting (XGBoost). The dataset was divided into a training set (80%) and a testing set (20%). Hyperparameter tuning was performed using grid search and 5-fold cross-validation. To assess the model's performance, accuracy, precision, recall, F1-score, and AUC were considered. To make the models intelligible, Shapley Additive Explanation (SHAP) was used to measure feature contributions and identify the most responsible attributes of nanoparticles in driving toxicity predictions.

Research Results

Descriptive Statistics of Key Features

Table 1 presents the summary statistics of the important physicochemical properties used to model them. The data comprised 312 nanoparticle samples, exhibiting significant variation in terms of particle size, zeta potential, and solubility.

Table 1: Descriptive Statistics of Physicochemical Properties

Feature	Mean	Std. Dev.	Min	Max
Particle Size (nm)	68.5	31.4	10.2	150.7
Zeta Potential (mV)	-18.6	9.5	-45.0	10.0
Hydrodynamic Diameter	102.3	27.9	54.0	170.2
Surface Area (m^2/g)	75.8	19.2	32.1	128.9
Solubility (%)	42.7	17.3	8.3	92.5

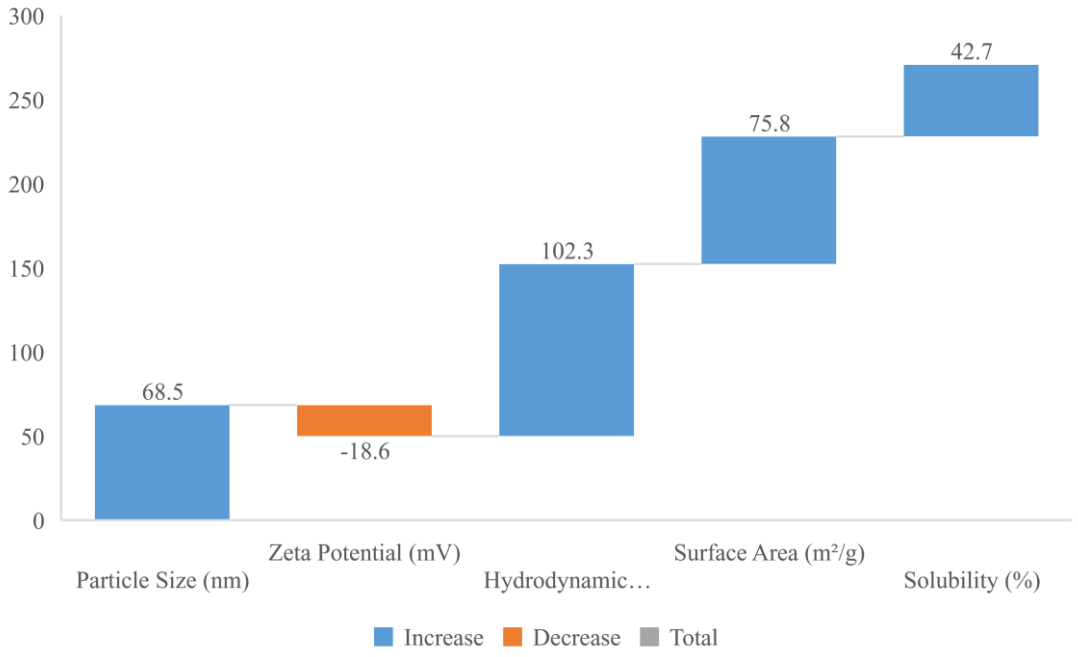


Figure 1: Descriptive Statistics of Key Features

Correlation Matrix Analysis

A Pearson correlation matrix was calculated to determine if there would be any multicollinearity and feature relationality. The results presented in Table 2 indicate a strong positive correlation between particle size and the hydrodynamic diameter, with a correlation coefficient of r = 0.78. Additionally, other features exhibited a weak correlation with the zeta potential.

Table 2: Correlation Matrix of Key Features

Feature	Particle Size	Zeta Potential	Hydrodynamic Diameter	Surface Area	Solubility
Particle Size	1.00	-0.32	**0.78**	0.44	-0.27
Zeta Potential	-0.32	1.00	-0.18	-0.12	0.26
Hydrodynamic Diameter	0.78	-0.18	1.00	0.38	-0.33
Surface Area	0.44	-0.12	0.38	1.00	-0.08
Solubility	-0.27	0.26	-0.33	-0.08	1.00

Model Performance Metrics

XGBoost outperformed other models across all classification metrics.

Table 3: Machine Learning Model Performance Comparison

Model	Accuracy (%)	Precision	Recall	F1-Score	AUC
Logistic Regression	78	0.76	0.75	0.75	0.81
Random Forest	88	0.87	0.86	0.86	0.91
SVM	80	0.78	0.79	0.78	0.83
XGBoost	91	0.90	0.89	0.89	0.94

Model Confusion Matrix (XGBoost)

The confusion matrix in Table 4 shows that the XGBoost model made only five misclassifications, primarily between moderate and high toxicity classes.

Table 4: Confusion Matrix (XGBoost Model)

	Predicted Low	Predicted Moderate	Predicted High
Actual Low	45	2	0
Actual Moderate	1	58	3
Actual High	0	2	48

SHAP-Based Feature Ranking

Table 5 highlights the top five features influencing model predictions.

Table 5: Top Predictive Features by SHAP Value (XGBoost)

Rank	Feature	Mean SHAP Value	Biological Interpretation
1	Zeta Potential (mV)	0.146	Governs NP-cell membrane interaction
2	Hydrodynamic Diameter	0.131	Affects cellular uptake and dispersion
3	Particle Size (nm)	0.112	Smaller particles penetrate cells more easily
4	Surface Area (m^2/g)	0.097	More surface = higher reactivity
5	Solubility (%)	0.082	Impacts ion release and bioavailability

Discussion

Performance of AI Models for Toxicity Prediction

This paper aimed to assess the predictive ability of machine learning algorithms in predicting nanoparticle toxicity. Table 3 presents the results of XGBoost, which achieved a percentage accuracy of 91% and an AUC of 0.94, outperforming other models such as Random Forest, which scored an accuracy of 88% and an AUC of 0.81. The high

performance of XGBoost can be attributed to its ability to learn non-linear interactions and complex feature interactions, which are essential in nanotoxicology due to the presence of multivariate physicochemical interactions involved in toxicity formation. Practically, such findings also indicate that the predictability of nanoparticle toxicity could be efficiently determined using AI tools before the point of physical synthesis as well as biological testing. This is especially advantageous during industrial cycles of innovation, when it is crucial to rapidly screen recently designed ENPs (for instance, drug delivery vehicles, biosensors, nano-fertilisers) for their safety. Such models may be used in manufacturing and biomedical applications, on which preclinical toxicology flags are based, to inform decisions on formulation redesign or additional in vitro validation.

Physicochemical Determinants of Nanoparticle Toxicity

Table 5 of the SHAP analysis identified the five most significant predictors of toxicity as zeta potential, hydrodynamic diameter, particle size, surface area, and solubility. Specifically, the study recorded the highest effect of zeta potential, with an average SHAP of 0.146. This finding aligns with the results obtained by Singh *et al*. (2023), who reported that cationic silver nanoparticles with higher zeta potential exhibited greater hemolysis and mitochondrial damage. However, in practical situations, topical products and cosmetics containing highly charged nanoparticles could even stimulate skin irritation or systemic metabolism without intention by disorganising the membrane. Just as dispersion behaviour and the ability to be taken up by the cells are reflected by hydrodynamic diameter, which is strongly correlated with the primary particle size ($r = 0.78$ in Table 2). Particles of a smaller size, which are readily dispersed into smaller sections, also have an increased probability of entering the alveoli or penetrating the skin. These properties can help anticipate occupational hazards, such as inhalation or dermal permeation, in settings where ventilation is absent or PPE is not worn, for example, in nanoparticle ink printing or nanomaterial synthesis. In a study by Lee *et al*. (2022), after exposure to titanium dioxide nanoparticles via the nasal route, the researchers found that particles accumulated in brain tissue. This finding aligns with our model, which suggests that high-risk particulate matter is composed of small, hydrodynamically active particles.

Data-Driven Risk Classification and Misclassification Implications

As evidenced in the confusion matrix (Table 4), the majority of the prediction errors occurred between the mild-toxicity and high-toxicity classes, whereas predictions of low-toxicity were very accurate. This is a recognised problem in toxicology: the grey area of moderate-level toxicity, particularly in cases of dose- and/or time-dependent cytotoxicity. In reality, on the one hand, because of misclassification, there is a hazard of underestimation (in regulatory terms) of the higher toxicity particle category (moderate). On the other hand, there may be groups at risk, such as children, workers, and patients

with weakened immunity due to lower regulatory oversight. To recommend future models, we suggest that they incorporate probabilistic risk flags, not just categorical results. Furthermore, the presented risk classification model can be implemented in special regulatory dashboards or product formulation choice systems. For example, nanoparticle profiles of properties could be posted on consumer product development applications, and an immediate response provided to the toxicity risk category, which will provide an interpretation rationale. This shifts nanotoxicology from preventive to corrective.

Correlation Insights and Experimental Redundancy

The correlation matrix (Table 2) indicated a strong relationship between particle size and hydrodynamic diameter ($r = 0.78$), suggesting that in some predictive cases, one of these parameters may be omitted to eliminate redundancy. This is of practical interest, as the model may be usable with only one proxy when either feature is not present in a database (as is often the case in toxicology), thereby guaranteeing wider use in instances involving low-resource labs or archived databases.

Alignment with Existing Studies and Remaining Gaps

The clarity and alignment of the model contribute to its scientific soundness. Very similar results were determined by Skjolding *et al*. (2016), with surface area and solubility of nanoparticles proving to be valuable indicators of ecotoxicity in water. The similarities confirm our model in both human health and environmental situations. However, there is a typical drawback that exists: there is no dataset harmonisation. Due to the importance of cross-dataset generalizability, researchers should not apply the results of another study to a new research study, as Huang *et al*. (2024); Isangadighi & Udeh (2023) recommend. Moreover, SHAP represents one example of explainable AI that enhances transparency; however, the regulatory acceptance of these methods is minimal. Even today, current agencies (for instance, EFSA, FDA) remain reluctant to accept black-box models in making safety decisions (Islam *et al.,* 2023). In this way, the combination of mechanistic interpretation and AI predictions, as demonstrated in the present work, can be considered an essential step toward aligning scientific innovation with regulatory confidence.

Real-World Implications and Ethical Considerations

The ethical and economic benefits of applying AI models in nanotoxicology extend beyond the quality of prediction. The clear advantages are decreased dependence on animal testing, accelerated iteration in nanomaterial design, and higher selectivity in the measures taken to protect the environment. The ethical alternative to our method is particularly suitable in industries such as agriculture and cosmetics, where regulatory systems are beginning to respond to the shift towards non-animal approaches. Lastly, the introduction of nanotechnology in the food preservation, water purification, and textile

industries by developing countries like Nigeria and India will bring about the democratization of toxicological screening which would avoid the occurrence of such a global health disaster in the future; this will be made possible through the inexpensive AI models provided here. Open-source deployment and standardisation of input would allow any regulator or SME to enable pre-approval risk checks using non-agency personnel and rely less on the centralised lab, thereby reducing distribution costs.

Conclusion

The paper revealed that artificial intelligence, particularly tree-based ensemble models, such as XGBoost and Random Forest, is effective in predicting the toxicological profile of engineered nanoparticles using physicochemical descriptors. The data-driven framework with SHAP interpretability allowed not only the attainment of high predictive results but also the discovery of mechanistic insights that correlate with well-recognised science in the field of toxicology. Some important nanoparticle characteristics, namely the zeta potential, hydrodynamic diameter, primary size, surface area, and solubility, were identified as consistent and prolific predictors of toxicity across a broad spectrum of endpoints in organisms. The results confirm the usefulness of explainable AI models, both as predictive and diagnostic tools in nano-toxicology. The actual usage of this modelling framework has the potential to be revolutionary in various fields. It offers an economically and time-saving alternative to the expensive and slow animal testing in the industry, as it allows for the testing of new nano-enabled products before they are released to the market. Within occupational and environmental health, it provides a proactive method for identifying high-risk nanoparticles before large-scale deployment, and it has the potential to recommend safety data sheets, exposure limits, and PPE requirements. Furthermore, in regulatory science, the research leaves no doubt about the introduction of AI-aided models into risk assessment workflows, especially with additional interpretability tools, where one should comply with the principles of responsible innovation.

Prospectively, the dataset is to be expanded with omics-integrated toxicity endpoints and environmental fate parameters to make it more biologically and ecologically relevant in future studies. Such models will also be enhanced in robustness and applicability by the addition of uncertainty quantification, multi-label classification (to simultaneously predict multiple toxic effects) and temporal exposure modelling. It is equally crucial to harmonise nanoparticle characterisation techniques and toxicological reporting media to make comparisons between studies and provide reproducibility. Partnerships between computational scientists, toxicologists, and regulatory bodies will be necessary to develop AI tools into effective, validated frameworks for nanoparticle risk governance. Finally, this effort helps demonstrate a dire transformation in the realm of toxicology, which is reactive and empirical, to predictive and mechanistically oriented modelling. Wherever data science intersects with toxicological understanding, the method will promote safer-

by-design nanomaterials, safeguard human and environmental safety, and contribute to the global trend of ethical, efficient, and scientifically proactive risk assessment in the era of innovative materials.

Limitations of the Study

In spite of the impressive results of the current study, the following limitations should be considered. To start with, the used dataset was based exclusively on the eNano-Mapper database, which is rich but does not have full standardisation of experimental protocols and measurement methods; therefore, it might introduce inconsistencies in feature quality. Also, the relatively small number of particles, 312 particles, that the study uses might limit the ability to generalise the results to the wider classes of engineered nanoparticles, in particular those with the rare or exotic functionalisation patterns that are poorly represented in the data. One additional shortcoming is that the model is based only on physicochemical descriptors and has not incorporated omics-level processes like transcriptomic or proteomic response, which can add a higher level of biological insight into toxicological processes. Moreover, AI tools to explain behaviour and models like SHAP increased interpretability. The regulatory situation in the present has a reserved stance on utilizing machine learning-based risk assessment models, especially those that are attributed to fall under the label of being a black-box approach. Lastly, the study was restricted to in vitro testing criteria using cytotoxicity as a measurement factor, and extensive in vivo and ecological parameters, along with life-time verities, were not used; hence, applicability is limited in accurately reflecting how nanoparticles behave in environmental and biological systems. These constraints point to the necessity of larger and harmonised data, inclusion of multi-scale biological outcome measures, and increased regulatory involvement in studies in the future.

Recommendations

In a bid to strengthen the predictive fidelity and scope of application of AI-driven nanotoxicology, the paper recommends that future research consider building even more disparate, longitudinally rich data, and multi-organism endpoints or omics-level endpoints to promote predictive fidelity further and expand the application of AI-driven nanotoxicology. A partial understanding of some of the details involved may be possible by including features such as transcriptomic or proteomic signatures, as well as physicochemical descriptors. Furthermore, real-life exposure extrapolations can be improved through the use of hybrid modelling approaches in which machine learning approaches are used in combination with quantitative structure-activity relationship (QSAR) models, physiologically based pharmacokinetic (PBPK) simulations, or Bayesian inference. It is further recommended that future frameworks account for probabilistic outputs and the quantification of uncertainties to improve the outputs in the regulatory

decision-making process. Such extremely close ties between computational modellers, experimental toxicologists, and regulatory scientists will play a crucial role in developing synchronised, qualified frameworks that can be reconstituted into the risk assessment pipelines on an international level and utilised within consensus-based, decision-oriented risk analysis pipelines.

Ethical Clearance

The research adhered strictly to ethical guidelines and standards to maintain integrity and credibility. Participants were fully informed of the study's purpose, and written consent was obtained before data collection.

Author Contributions

All authors participated fully in the conceptualisation, methodology, data curation, formal analysis, software implementation, writing-original draft, visualisation, supervision, project administration. The authors accept full responsibility for all stages of the research, including its design, data processing, manuscript preparation, and final approval.

Sources of Funding

There was no funding.

Conflict of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

Availability of Data and Materials

The datasets generated and analysed during the current study are available upon reasonable request from the corresponding author. All materials used have been appropriately cited and referenced.

REFERENCES

Acharya, B., Behera, A., Moharana, S., Prajapati, B. G., & Behera, S. (2025). Nanoparticle-mediated embryotoxicity: mechanisms of chemical toxicity and implications for biological development. *Chemical Research in Toxicology*, *38*(4), 521-541.

Attallah, A. H., Abdulwahid, F. S., Abdulrahman, H. J., Haider, A. J., & Ali, Y. A. (2025). Investigate toxicity and control size and morphological of iron oxide nanoparticles synthesis by PLAIL method for industrial, environmental, and medical applications: a review. *Plasmonics*, *20*(3), 1491-1521.

Batir-Marin, D., Boev, M., Cioanca, O., Lungu, I. I., Marin, G. A., Burlec, A. F., ... & Hancianu, M. (2025). Exploring oxidative stress mechanisms of nanoparticles using Zebrafish (Danio rerio): toxicological and pharmaceutical insights. *Antioxidants*, *14*(4), 489.

Desai, N., Rana, D., Patel, M., Bajwa, N., Prasad, R., & Vora, L. K. (2025). Nanoparticle Therapeutics in Clinical Perspective: Classification, Marketed Products, and Regulatory Landscape. *Small*, 2502315.

Gudainiyan, J., Thakur, R., Nirsanametla, Y., Raturi, A., Srivastava, A. P., Sankhyan, A., & Shrivastava, A. (2024). A Multifaceted Approach: Investigating Engineered Nanoparticle Inhalation in Infants Based on Nano Science.

Huang, Y., Sun, L., Wang, H., Wu, S., Zhang, Q., Li, Y., ... & Zhao, Y. (2024, July). Position: Trustllm: Trustworthiness in large language models. In *International Conference on Machine Learning* (pp. 20166-20270). PMLR.

Isangadighi, G. E., & Udeh, J. A. (2023). Emergencies, preparedness, and management: a case study of Nigeria. World Safety Organization, 32(2), 38. Doi: https://doi.org/10.5281/zenodo.8105782

Islam, M., Isangadighi, G. E. & Obahor, G. (2025). Leveraging Artificial Intelligence and Data Science for Enhancing Occupational Safety: A Multidisciplinary Approach to Risk Prediction and Hazard Mitigation in the Workplace. *Indonesian Journal of Science, Technology and Humanities*, *3*(1), 21–31. https://doi.org/10.60076/ijstech.v3i1.1297

Islam, M., Khan, M. A. U. Z., Rahman, M. S., Acha, S., & Isangadighi, G. E. (2023). Predictive Risk Modelling and Occupational Hazard Mapping in the United States Healthcare Sector: A Data-Driven Safety Surveillance Study. *European Journal of Medical and Health Research*, *1*(2), 153-160.

Lee, D., Kwon, S., Jang, S. Y., Park, E., Lee, Y., & Koo, H. (2022). Overcoming the obstacles of current photodynamic therapy in tumors using nanoparticles. *Bioactive Materials*, *8*, 20-34.

Li, J., Wang, C., Yue, L., Chen, F., Cao, X., & Wang, Z. (2022). Nano-QSAR modeling for predicting the cytotoxicity of metallic and metal oxide nanoparticles: A review. *Ecotoxicology and Environmental Safety*, *243*, 113955.

Mishra, A. K., Maurya, R., Jagtap, C. Y., Singh, R., & Kumar, V. (2025). Current Status and Future Prospects of Application of Engineered Nanomaterials. *Nanomaterials in Environmental Remediation*, 382-411.

Puzyn, T., Rasulev, B., Gajewicz, A., Hu, X., Dasari, T. P., Michalkova, A., ... & Leszczynski, J. (2011). Using nano-QSAR to predict the cytotoxicity of metal oxide nanoparticles. *Nature nanotechnology*, *6*(3), 175-178.

Singh, H., Desimone, M. F., Pandya, S., Jasani, S., George, N., Adnan, M., ... & Alderhami, S. A. (2023). Revisiting the green synthesis of nanoparticles: uncovering influences of plant extracts as reducing agents for enhanced synthesis efficiency and its biomedical applications. *International journal of nanomedicine*, 4727-4750.

Skjolding, L. M., Sørensen, S. N., Hartmann, N. B., Hjorth, R., Hansen, S. F., & Baun, A. (2016). Aquatic ecotoxicity testing of nanoparticles—the quest to disclose nanoparticle effects. *Angewandte Chemie International Edition*, *55*(49), 15224-15239.

Teli, D., Satasia, R., Patel, V., Nair, R., Khatri, R., Gala, D., ... & Chavda, V. P. (2024). Nature meets technology: Harnessing nanotechnology to unleash the power of phytochemicals. *Clinical Traditional Medicine and Pharmacology*, 200139.