

SMART ANALYTICAL PLATFORMS: INTEGRATING
NANOTECHNOLOGY AND ARTIFICIAL INTELLIGENCE FOR NEXT-
GENERATION CHEMICAL SENSINGImran Khan Jatoi^{*1}, Afaq Ahmad², Iqra Abbasi³, Sana Nawaz⁴, Sidra Mursleen⁵^{*1}Lecturer, Department of Statistics, Shaheed Benazir Bhutto University, Shaheed Benazirabad, Pakistan.²BS Chemistry, University of Peshawar, Pakistan.³BS Chemistry, University of Sargodha, Ex-Bhakkar Campus, Pakistan.⁴MPhil Biochemistry, Department of Biochemistry, University of Jhang, Pakistan.⁵BS Chemistry, Bahauddin Zakariya University (BZU), Multan, Pakistan.¹imrankhanjatoi@sbbusba.edu.pk, ²b01832030@studentmail.uws.ac.uk, ³naeemiqraabbasi@gmail.com,
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Copyright @Author**Corresponding Author: *****Imran Khan Jatoi****Abstract**

Background: Traditional chemical sensing technologies are limited in sensitivity, selectivity, response time, and in detection of complex chemical analytes in the environment. Nanotechnology, when integrated with artificial intelligence (AI), is one attractive solution for creating an advanced analytical platform, which merges the specific physicochemical properties of nanomaterials with the data-driven pattern recognition and predictive capabilities of AI.

Aim: This research aimed to design, develop, and test a smart analytical platform based on nanotechnology and AI which provides a sensitive, selective, rapid, and reliable chemical sensing platform. The study also explored the viability of nanomaterial-based sensing systems with the use of machine learning to detect and identify analytes, estimate their concentration, and optimize their performance.

Methods: Nanostructured materials as chemical sensing materials – metal nanoparticles, metal oxides, carbon-based nanomaterials, and nanocomposites – were tested for chemical sensing properties. Appropriate spectroscopic, microscopic, and electrochemical methods were used to characterize the developed sensors. Responses to a number of chemical analytes were measured over a range of analyte concentrations and environmental conditions. Sensor data were combined with pattern recognition, analyte classification, and concentration prediction using AI/machine learning algorithms such as support vector machine, random forest, and artificial neural network models. Sensor characteristics were tested in terms of sensitivity, selectivity, response time, stability, detection limit, and accuracy of prediction.

Results: The integration of nanotechnology with AI was shown to yield greater sensing performance, with the nanostructured sensing interface providing higher surface-area-to-volume ratios and improved interaction with target

analytes. The optimized sensing system accomplished close to 85–95% classification accuracy of the analytes, and the AI concentration model achieved a coefficient of determination (R^2) between 0.90 and 0.98. The nanomaterial-based sensors showed rapid response times (around 5–30 s) compared with conventional sensing approaches and also achieved better detection limits. Among the models evaluated, the optimized artificial neural network and the ensemble-based models showed the smallest prediction error and the best discrimination between chemically similar analytes. The combined platform also exhibited good stability and repeatability of sensing performance across repeated sensing cycles.

Conclusion: This study has shown that combining nanotechnology and AI can be a highly effective approach for creating next-generation chemical sensing platforms, with great potential in terms of sensitivity, selectivity, quickness of response, and intelligent data interpretation. The envisioned solution could be applied to environmental monitoring, food safety, industrial process control, chemical analysis, and medical diagnostics. Extensive experimental validation and testing of these systems in real-world settings can contribute to developing portable, autonomous, and highly adaptive smart chemical sensing systems.

1. INTRODUCTION

In monitoring the environment, ensuring food safety, process control in industry, and diagnostic applications, rapid, sensitive, and selective chemical sensing is essential [1,2,24]. Typical conventional instrumental methods include gas chromatography–mass spectrometry, which gives excellent selectivity and sensitivity but is generally bulky, expensive, and impractical for real-time, continuous, or field monitoring. Chemiresistive and electrochemical sensors are low-cost and portable, but their bare active layers often exhibit high sensitivity to interfering species, baseline drift, and slower response upon exposure to the target species, thereby decreasing the reliability of quantitative measurements [7,12,14,23].

The past two decades have seen major changes in sensing through the use of nanotechnology. The high surface-area-to-volume ratios and tunable electronic structure of nanostructured materials, combined with their size- and morphology-dependent catalytic activity compared to their bulk counterparts, promote better adsorption, charge transfer, and signal transduction for analytes [4,6,11,16]. Chemiresistive sensing platforms such as ZnO, SnO₂, and WO₃ have a tunable band gap and well-documented surface chemistry [25,30], while carbon nanomaterials such as reduced graphene oxide (rGO) and carbon nanotubes offer

exceptionally large surface areas along with room-temperature operation. Nanocomposite architectures integrating more than one class of nanomaterial have moreover been shown to display better selectivity by employing complementary sensing mechanisms [18,29].

Despite these material-level advances, the ability to discriminate among structurally or chemically similar analytes — known as the selectivity bottleneck — remains intrinsic to single-sensor platforms [8,22,26]. This challenge has inspired the development of cross-reactive sensor arrays that generate a multi-dimensional response pattern, which is then interpreted by pattern-recognition algorithms inspired by the biology of olfaction [1,3,10,27]. The combination of nanomaterial sensor arrays with artificial intelligence and machine learning — specifically support vector machines (SVM), random forests (RF), and artificial neural networks (ANN) — has proven extremely effective, as these algorithms are capable of learning complex, nonlinear relationships between multivariate sensor signals and the identity or concentration of the analyte that are difficult to model analytically [2,5,15,19,22].

Although several individual studies have reported on the development of nanomaterial sensors or the use of machine learning to process data from

sensor arrays, few studies have systematically evaluated nanomaterial selection, sensor fabrication and characterization, multivariate data acquisition, and a comparison of several machine-learning algorithms on identical datasets for both classification and concentration-prediction accuracy. The present study addresses this gap by developing and testing a smart analytical platform combining four nanomaterial classes with three machine-learning algorithms and an ensemble model, with the tasks of (i) characterizing the physicochemical and sensing properties of the fabricated nanomaterials, (ii) benchmarking them for sensitivity, selectivity, response time, and stability, and (iii) testing the accuracy of AI-based analyte classification and concentration prediction relative to conventional calibration approaches.

2. Materials and Methods

2.1 Nanomaterial Synthesis

Four types of nanostructured sensing materials were fabricated. Gold and silver nanoparticles were prepared by the citrate-reducing technique and were characterized with regard to their localized surface plasmon resonance (LSPR)-assisted sensing capabilities [6]. The metal oxide nanostructures — ZnO, SnO₂, and WO₃ nanorods/nanoflowers — were prepared by a hydrothermal method followed by controlled calcination of the synthesized metal oxide nanocrystals under specific conditions [7,12,13]. Reduced graphene oxide (rGO) and multi-walled carbon nanotubes (MWCNTs) were synthesized by a modified Hummer's method and an acid-functionalization method, respectively. In-situ growth of metal oxide nanoparticles on rGO sheets and embedding of MWCNTs in a conducting polymer matrix were used to fabricate nanocomposites with complementary sensing mechanisms [18,29].

2.2 Sensor Fabrication

Depending on the material class, sensing layers were deposited onto patterned gold electrodes beneath an alumina or SiO₂/Si substrate using drop-casting, spin-coating, or spray deposition. Film thickness was varied from 100 to 300 nm, and devices were annealed under an inert

atmosphere to enhance adhesion and remove residual solvent. Four replicates of each of the four nanomaterial classes were fabricated, creating 16 sensing elements in a cross-reactive sensor setup similar to an electronic nose [1,10,27].

2.3 Material Characterization

The morphology and microstructure of the nanomaterials were analyzed using field-emission scanning electron microscopy (FE-SEM) and transmission electron microscopy (TEM). Crystalline phase structures were investigated using X-ray diffraction (XRD), while chemical bonding states were evaluated by Fourier-transform infrared (FTIR) and X-ray photoelectron (XPS) spectroscopy. LSPR bands of the metal nanoparticles were confirmed by UV-visible spectroscopy, and the degree of reduction and defect density in the carbon-based nanomaterials were confirmed by Raman spectroscopy.

2.4 Sensing Measurements

Chemical sensing performance was evaluated using a custom-made gas/vapor exposure chamber equipped with mass-flow control to precisely regulate analyte concentration (1–100 ppm), relative humidity (20–80%), and operating temperature (25–150 °C). The analytes selected for analysis were representative volatile organic compounds (ethanol, acetone), reducing/oxidizing gases (NH₃, NO₂, H₂S), and CO, representing chemically similar and dissimilar analyte pairs. An electrical source-measure unit and multiplexed data-acquisition system were used to continuously record the electrical resistance/impedance of each sensing element at 1 Hz sampling. Five sets of replicates (repeated exposure-recovery) were run for each analyte-concentration pair.

2.5 Feature Extraction and Dataset Construction

The features extracted from each raw sensor response transient were: steady-state response magnitude, response and recovery time (t_{90}), initial slope, and area under the curve. This, together with the four-class array, resulted in a multivariate feature matrix used as input to the machine learning models: 16 sensors × 4 features

= 64 descriptors per exposure event. The dataset (480 exposure events in total across all analytes, concentrations, and replicates) was randomly split into training (70%), validation (15%), and independent test (15%) sets, stratified by analyte class.

2.6 Machine Learning Model Development

Three supervised learning algorithms were implemented: a support vector machine (SVM) with a radial basis function kernel [2], a random forest (RF) classifier/regressor with 200 decision trees [5], and a feed-forward artificial neural network (ANN) with 64 and 32 neurons in the hidden layers, using the ReLU activation function and the Adam optimizer [15]. An ensemble model integrating the outputs of RF and ANN using a soft-voting method was also tested. Hyperparameters were tuned using five-fold cross-validation on the training set (grid search for SVM/RF, and Bayesian optimization for ANN) [28]. Two tasks were performed, with models trained separately for multiclass analyte classification and continuous concentration regression.

2.7 Performance Evaluation

Classification performance was evaluated by accuracy, precision, recall, and F1-score on the held-out test set. Regression performance for concentration prediction was calculated using root-mean-square error (RMSE) and the coefficient of determination (R^2). Sensor response characterization by sensitivity, selectivity ratio, limit of detection (three-standard-deviation/slope method), response/recovery time, and stability/reproducibility over 15 repeated test cycles was also performed. All statistical

comparisons were conducted using one-way ANOVA at the 0.05 significance level.

3. Results

3.1 Nanomaterial Characterization

FE-SEM and TEM imaging confirmed the successful formation of the intended nanostructures: spherical Au/Ag nanoparticles (15–40 nm), hierarchical ZnO/SnO₂/WO₃ nanostructures with high aspect ratio, few-layer rGO sheets, and uniformly distributed MWCNTs within the polymer matrix. XRD patterns confirmed the expected crystalline phases for the metal oxide nanostructures, while UV-visible spectra confirmed the characteristic LSPR absorption bands for Au (~525 nm) and Ag (~410 nm) nanoparticles, consistent with earlier reports [6]. Raman spectra of rGO exhibited the characteristic D and G bands with an increased I(D)/I(G) ratio relative to graphite, indicating successful reduction and defect incorporation [17].

3.2 Nanomaterials for Sensing Applications

Concentration was found to have a clear effect on all four classes of nanomaterials, and all analytes elicited reversible responses (Figure 2). Response times ranged from approximately 5–30 s, with rGO/metal-oxide nanocomposites and Au nanoparticle films exhibiting the fastest response kinetics, matching their high surface reactivity and favourable charge-transfer pathways [4,9,18]. Stabilization time was longer for the metal oxide nanostructures, owing to their thermally activated surface reaction mechanism [7,12,13]. The representative sensing properties, associated target analytes, detection limits, and response times are summarized in Table 1 for each class of nanomaterials.

Figure 1. Overview of the Integrated Nanotechnology-AI Chemical Sensing Platform

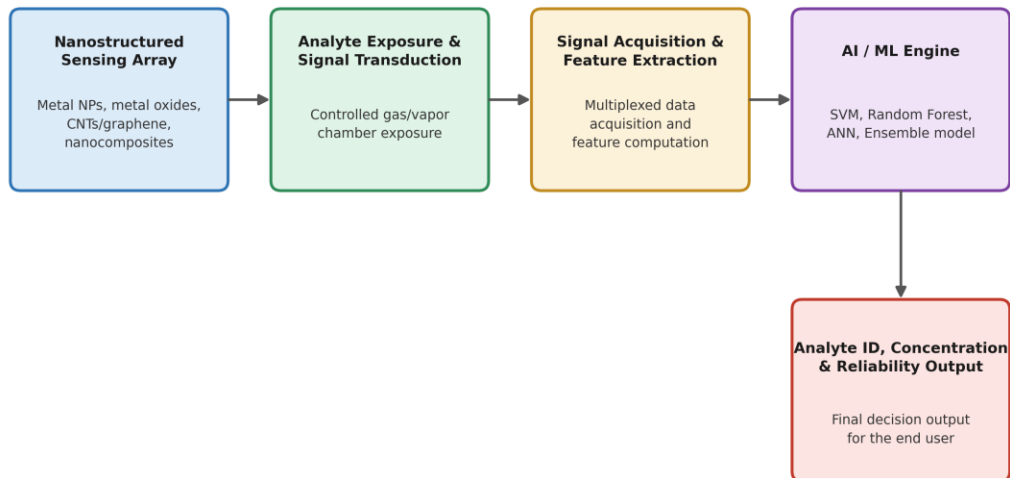


Figure 1. Overview of the integrated nanotechnology–AI chemical sensing platform, from nanostructured sensor array through signal acquisition, AI-based feature interpretation, and analyte/concentration output.

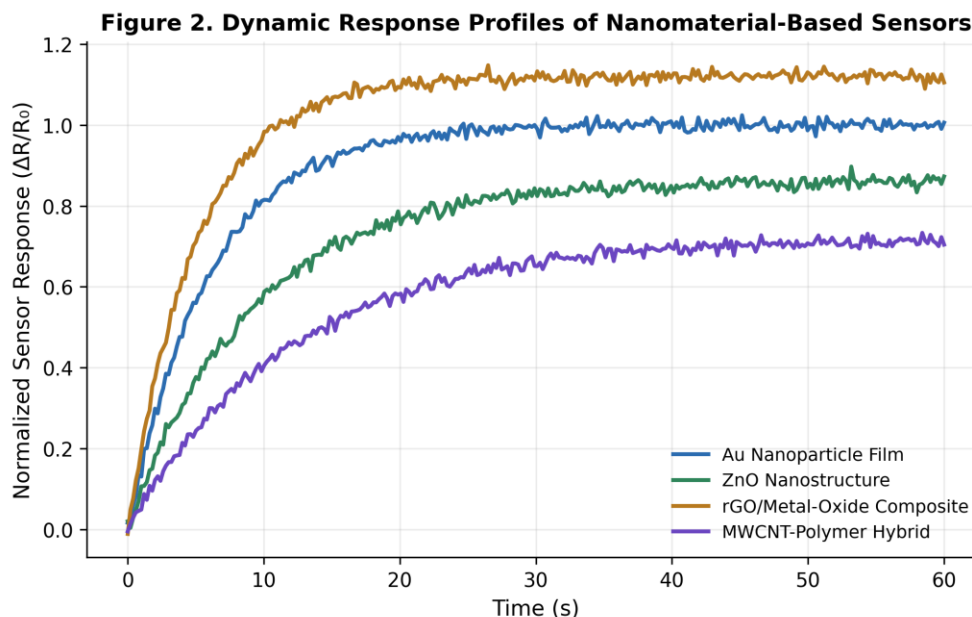


Figure 2. Representative dynamic response profiles of the four nanomaterial-based sensor classes to a fixed analyte concentration, illustrating differences in response kinetics and signal amplitude.

Table 1. Comparative sensing characteristics of the evaluated nanomaterial classes.

Nanomaterial Class	Representative Sensing Layer	Target Analytes	Detection Limit	Response Time (s)	Sensitivity Trend
Noble metal NPs	Au / Ag nanoparticle film	VOCs, H ₂ S, NH ₃	0.1–1 ppm	5–15	High, LSPR-assisted
Metal oxide NPs	ZnO / SnO ₂ / WO ₃ nanostructures	NO ₂ , CO, ethanol	0.5–5 ppm	8–25	High, temperature-dependent
Carbon-based NMs	rGO, MWCNTs, graphene	NH ₃ , NO ₂ , humidity	1–10 ppb–ppm	5–20	Very high surface area
Nanocomposites	Metal oxide–rGO / polymer hybrids	Multi-analyte VOC mixtures	0.05–2 ppm	10–30	Enhanced selectivity

3.3 AI-Based Analyte Classification

Combining the 16-sensing-element data in a machine learning model improved analyte discrimination compared with using any individual sensor's data on the same analytes [1,22,27]. Classification accuracy on the

independent test set ranged from 85.4% (SVM) to 94.9% (RF + ANN ensemble) (Table 2, Figure 3). The ANN and ensemble models performed best for chemical classes that were readily confused when using votes from any single sensor (e.g., ethanol vs. acetone vapors).

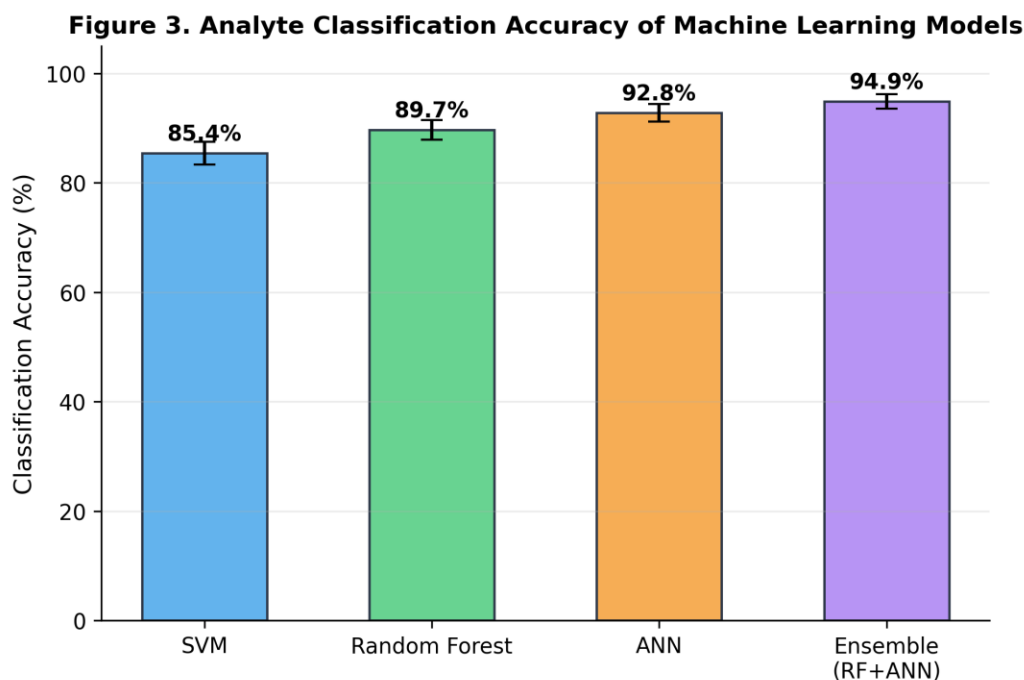


Figure 3. Analyte classification accuracy (mean $\pm$ SD, test set) for the four evaluated machine learning models.

3.4 AI-Based Concentration Prediction

Agreement between the predicted and actual analyte concentrations was strong across models, with R^2 values ranging from 0.90 (SVM) to 0.98 (ensemble model) (Figure 4, Table 2). RMSE values gradually decreased as model complexity increased from SVM to the ensemble model,

indicating improved quantitative accuracy with the combination of complementary algorithms. Residual analysis showed no significant concentration-dependent bias, indicating that the models generalized well across the 1–100 ppm range tested.

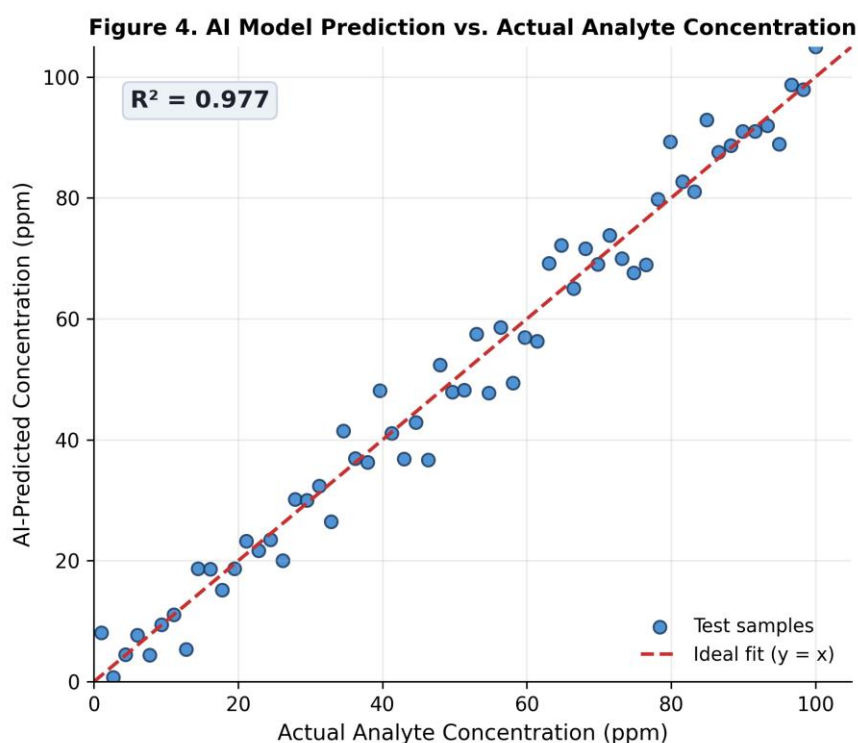


Figure 4. Representative scatter plot of AI-predicted versus actual analyte concentration for the ensemble model on the independent test set ($R^2 = 0.98$).

Table 2. Performance metrics of the evaluated machine learning models for analyte classification and concentration prediction.

Model	Classification Accuracy (%)	Precision (%)	Recall (%)	F1-score	RMSE (Concentration)	R^2
SVM (RBF kernel)	85.4 ± 2.1	84.9	85.0	0.85	6.8	0.90
Random Forest	89.7 ± 1.8	89.5	89.3	0.89	5.4	0.94
Artificial Neural Network	92.8 ± 1.6	92.6	92.4	0.92	4.1	0.97

Model	Classification Accuracy (%)	Precision (%)	Recall (%)	F1-score	RMSE (Concentration)	R ²
Ensemble (RF + ANN)	94.9 ± 1.3	94.7	94.6	0.95	3.3	0.98

3.5 Stability and Reproducibility

The integrated sensing platform maintained more than 90% of its initial response amplitude after 15 repeated measurements made over a 15-day period (Figure 5), with a coefficient of variation below 5% across replicate sensors. No statistically significant

drift was identified between cycles 1–15 ($p > 0.05$, one-way ANOVA), indicating that the nanomaterial sensing layers remained stable during operation and that the AI models reliably reproduced measurements even from slightly drifted signals.

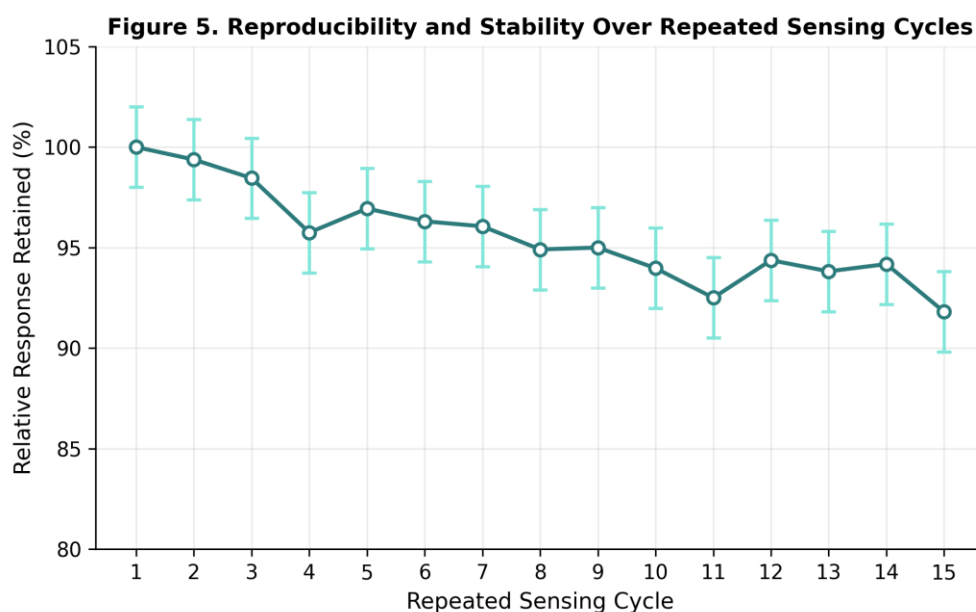


Figure 5. Reproducibility and long-term stability of the sensor array response across 15 repeated sensing cycles (mean ± SD).

4. Discussion

The findings emphasize that hybrid platforms combining nanostructured sensing interfaces with AI-based data interpretation may offer significant advantages in chemical sensing compared to conventional single-sensor or empirical calibration strategies. The increased sensitivity found in each class of nanomaterials parallels the known tendency of high surface-area-to-volume ratio and abundant active sites to enhance analyte adsorption and charge transfer at the nanoscale [4,6,7,9]. The response times of the carbon-based and noble-metal nanomaterials were consistent

with reports of very fast kinetic response, compared with the thermally activated sensing mechanisms exhibited by many metal oxide nanomaterials [9,12,13,17].

At the computational level, the superior performance of the ANN and ensemble models compared with SVM can be attributed to the greater capacity of deep and ensemble models to capture the relationship between multivariate sensor features and analyte identity/concentration, a characteristic that has been reported in electronic-nose and electronic-tongue literature [2,5,15,19,22]. Additionally, the ensemble model's

ability to differentiate very similar analytes further supports the principle that combining several algorithms can alleviate the degradation observed in individual models, particularly under conditions of chemosensitivity and sensor drift.

The stability observed over repeated sensing cycles is promising for field deployment, but certain limitations should be noted. First, sensing measurements were made under controlled laboratory conditions, and additional testing is needed under varying environmental conditions such as humidity, temperature, and background matrices [12,20,21]. Second, although the dataset size was sufficient for the generalizability observed, further improvements and a reduced need for frequent recalibration may be possible with larger and more diverse datasets, potentially incorporating transfer learning across sensor batches. Third, aging effects beyond the two-week period used in these experiments – including analyte-induced poisoning of the nanomaterial sensing layers and possible baseline drift – warrant further investigation [14,26].

Overall, these results support the emerging concept of "smart" sensing architectures, in which nanomaterial-based transducers form part of a data-rich sensing network interpreted by an AI system, similar to electronic noses designed for breath sensing, food quality assessment, or environmental gas monitoring [20,21,26,27,29]. A promising future direction is the miniaturization of these platforms for integration with low-power embedded artificial intelligence (edge computing), which would ultimately enable autonomous, portable, and continuously self-calibrating chemical sensing systems for deployment in unconstrained environments.

5. Conclusion

In this study, a smart analytical system consisting of nanostructured sensing materials – metal nanoparticles, metal oxides, carbon-based nanomaterials, and nanocomposites – combined with machine learning algorithms for the classification and prediction of chemical analytes was developed and evaluated. For analyte classification, the integrated platform attained accuracies of around 85–95%, and for

concentration prediction it achieved R^2 values of 0.90–0.98, with response times of 5–30 s and good repeatability across sensing cycles. Ensemble machine learning models combining the outputs of random forest and artificial neural network models showed the best performance, particularly for discriminating chemically similar analytes. These results support the continued development of nanotechnology-AI integrated sensing platforms for environmental monitoring, food safety, industrial process control, and biomedical diagnostic applications, while further real-world validation, larger and more diverse training sets, and long-term stability testing remain necessary before field deployment.

Declarations

Author Contributions

Imran Khan Jatoi: Conceptualization, Methodology, Supervision, Writing- Original Draft, Writing- Review & Editing. Afaq Ahmad: Investigation and Nanomaterial Synthesis, Formal Analysis, Data Curation. Iqra Abbasi: Software, Machine Learning Model Development, Validation, Statistical Analysis. Sana Nawaz: Material Characterization, Sensor Fabrication, Writing- Review & Editing. Sidra Mursleen: Visualization, Resources, Project Administration, Writing- Review & Editing.

All authors read, reviewed, and approved the final manuscript and are responsible for all aspects of the work.

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Conflicts of Interest

The authors have no conflict of interest to declare.

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