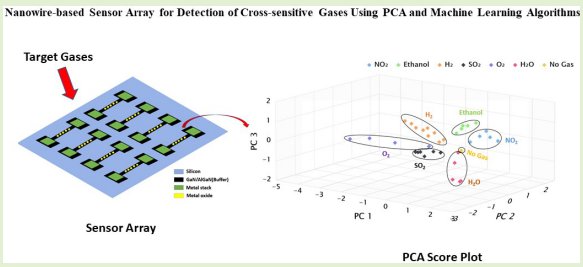
Nanowire-Based Sensor Array for Detection of Cross-Sensitive Gases Using PCA and Machine Learning Algorithms

Md Ashfaque Hossain Khan, Brian Thomson, Ratan Debnath, Abhishek Motayed, and Mulpuri V. Rao

***Abstract*—In this work, a gas sensor array has been designed and developed comprising of Pt, Cu and Ag decorated TiO_2 and ZnO functionalized GaN nanowires using industry standard top-down fabrication approach. The receptor metal/metal-oxide combinations within the array have been determined from our prior molecular simulation results using first principle calculations based on density functional theory (DFT). The gas sensing data was collected for both singular and mixture of NO_2, ethanol, SO_2 and H_2 in presence of H_2O and O_2 gases under UV light at room temperature. Each gas produced a unique response pattern across the sensors within the array by which precise identification of cross-sensitive gases is possible. After pre-processing of raw data, unsupervised principal component analysis (PCA) technique was applied on the array response. It is found that, each analyte gas forms a separate cluster in the score plot for all the target gases and their mixtures, indicating a clear discrimination among them. Then, four supervised machine learning algorithms such as- Decision Tree, Support Vector Machine (SVM), Naive Bayes (kernel) and k-Nearest Neighbor (k-NN) were trained and optimized using their significant parameters with our array dataset for the classification of gas type. Results indicate that the optimized SVM and NB classifier models exhibited 100% classification accuracy on test dataset. Practical applicability of the considered algorithms has been discussed as well. Moreover, this array device works at room-temperature using very low power and low-cost UV light-emitting diode (LED) as compared to high power consuming commercially available metal-oxide sensors.**



***Index Terms*—Sensor array, cross-sensitivity, gas sensor, principal component analysis (PCA), machine learning.**

I. Introduction

THERE is a great need for the development of highly selective sensors for detecting various toxic gases and their mixtures in many industrial, medical, space exploration and environmental monitoring applications. Environmental gases such as SO_2, NO_2, ethanol and H_2 are harmful either to the environment and/or to living beings and their monitoring requires sensors capable of detecting ppm level of these gases well below their Occupational Safety and Health Act (OSHA) permissible exposure limits [1]. Metal oxide-based sensors to detect these environmental pollutants have been the subject of intensive research for several decades [2]. However, these metal oxide sensors lack precise selectivity towards any specific gas. Their mechanism of sensing involves chemical interaction of the analyte with the oxygen chemisorbed on the surface [3]. The cross-sensitivity among different analytes is unavoidable, irrespective of their oxidizing or reducing nature. Systematic variations in the parameters such as dopants, additives, operating temperatures, bias voltage, grain size and morphology were adopted to achieve the necessary selectivity among various analytes [4]. Though the efforts had been made, the problem of cross-sensitivity for a single metal oxide-based sensor can't be fully eliminated.

With the advancement in nano fabrication and chip integration, there exists a tremendous opportunity for developing an integrated chip comprising of several nano sensors that can differentiate among the analyte types [5]. This integrated sensor chip would be able to discriminate the toxic gases which exhibit similar charge transfer process during adsorption and desorption.

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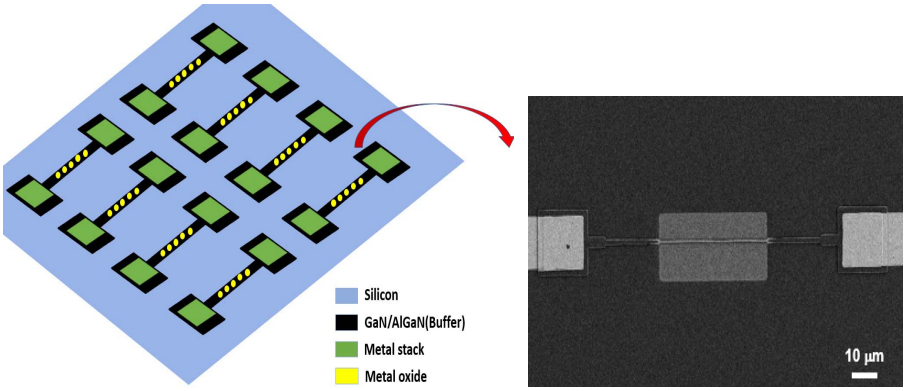

Fig. 1. (Left) Schematic of a sensor array containing eight metal/metal-oxide functionalized GaN nanowires. (Right) FESEM image of an individual nanowire sensor.

In this paper, we have presented a sensor array comprised of eight different metal/metal-oxide functionalized GaN nanowire sensors mounted on a PCB which can produce unique response pattern for each target gas. We used Pt, Cu and Ag decorated TiO_2 and ZnO on GaN surface for the detection of NO_2, ethanol, SO_2, H_2 and their mixtures in the presence of H_2O and O_2 gases at room temperature (20 °C). The sensor array data was acquired for both singular and mixture of gases which were pre-processed using RapidMiner software. Then, unsupervised principal component analysis (PCA) technique was applied on the array response for precise identification of those target gases. Furthermore, four different supervised machine learning algorithms such as- decision tree, support vector machine, naive Bayes (kernel) and k-Nearest Neighbor were optimized for our dataset. The performance of these classifiers had been studied to find out the suitable algorithm for gas classification. The proposed array device works at room-temperature using only a low power (micro-watt), and low-cost commercial UV light-emitting diode (LED) as compared to high power consuming commercially available metal-oxide sensors.

II. Experimental

A. Sensor Array Fabrication

The sensing elements of the sensor array are composed of metal/metal-oxide function-alized GaN nanowires (Figure 1). The nanowire-based sensors have been fabricated using the standard top-down fabrication technique in a class 100 clean-room. Si-doped GaN nanowires having a width of 300-400 nm were formed on silicon substrate by production standard stepper lithography assisted inductively coupled plasma (ICP) etching of GaN epilayer grown on Si substrate. Ohmic metal contacts were formed on nanowire ends with a deposition sequence of Ti (40 nm)/Al (80 nm)/Ti (40 nm)/Au (40 nm) in a standard electron beam evaporator. After that, SiO_2 layer was deposited on the device by plasma-enhanced chemical vapor deposition (PECVD) to protect the nanowire and metal contacts from being damaged during high temperature processing and etching. The details of the device fabrication including the schematic process flow diagram can be found in our previous papers [6], [7]. Reactive ion etching (RIE) was employed to create an active area on GaN nanowire for the metal/metal-oxide nanoclusters functionalization. A thin layer (5-10 nm) of TiO_2 or ZnO were deposited on nanowire surface by RF magnetron sputtering in a reactive atmosphere with O_2 flow at 40 °C and 280 W RF power. Then, rapid thermal annealing (RTA) was performed in pure Ar at 600-700 °C for 4-5 mins in order to crystallize the deposited metal oxides and to enhance the ohmic contacts to the GaN nanowires. Next, receptor metals such as- Pt, Cu and Ag were added on top of metal-oxide by e-beam evaporation with a deposition rate of 1-1.5 Å/s. The typical thickness of these metals is 1-5 nm. Thus, we got a total of eight metal/metal-oxide combinations, including the bare metal-oxides on GaN nanowires. The receptor metal/metal-oxide combina- tions for the target gases have been chosen from our previous molecular simulation results using first principle calculations based on density functional theory (DFT) [8]. After the deposition of Ti/Au metal bond pads on the ohmic contacts, sensor devices were mounted on and wire bonded to leadless chip carrier (LCC) packages. Then, all these eight different metal/metal-oxide functionalized sensor devices have been mounted and integrated into a pre-designed printed circuit board (PCB) to develop the final sensor array device.

B. Instruments and Experimental Set-Up

The current-voltage measurements of the fabricated devices were performed by a National Instrument (NI) PXI SMU system under a LED UV light source having a wavelength of 365 nm and output power of 470 mW/cm^2. The sensor array was placed in a custom designed gas chamber made of stainless steel for gas sensing data collection. A mixture of target gases and compressed breathing air was flowed into the sensing chamber and the net flow (air + analytes) was maintained at 0.5 slpm. Mass flow controllers (MFCs) independently controlled the flow rate of each component, determining the composition of the mixed gas. The sensor array currents were collected by the NI PXI SMU system at a constant 5V DC voltage. The devices have been allowed to regain the baseline current without purging the gas chamber after exposure. Sensor response was calculated as $(R_{gas} - R_{air})/R_{air}$, where R_{gas} and R_{air} are the resistances of the sensor in

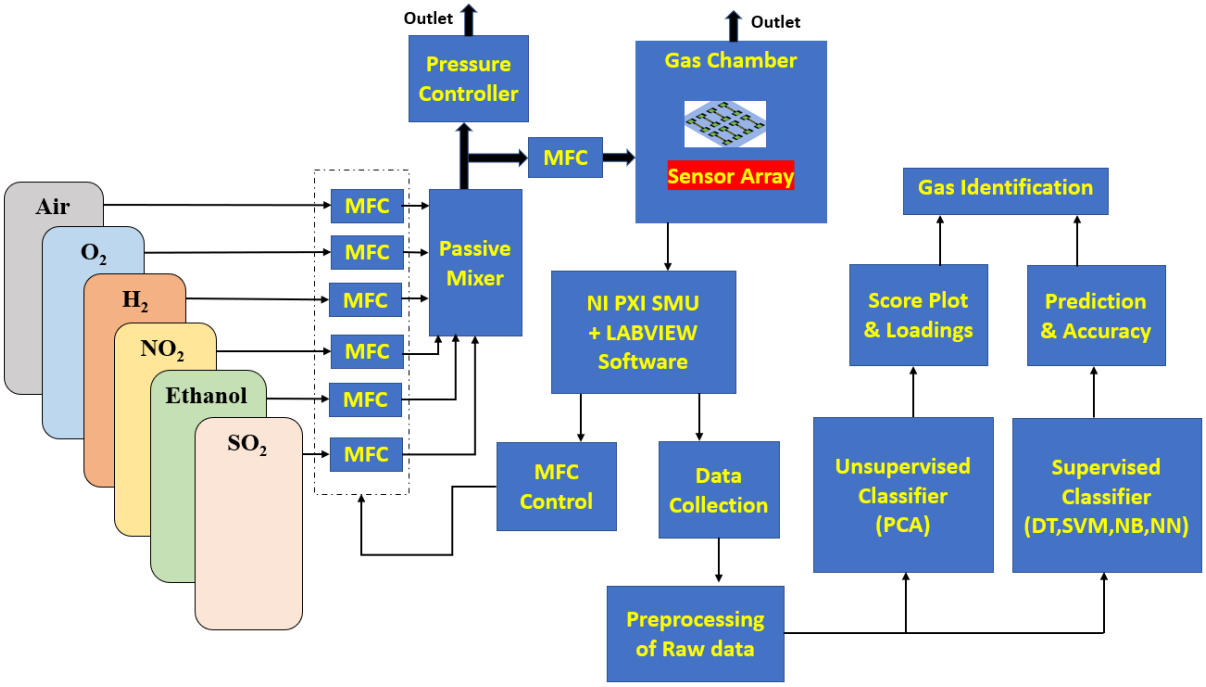

Fig. 2. The process flow for the gas sensing data collection and analysis.

the presence of the analyte–air mixture and in the presence of air, respectively. Figure 2 illustrates the process flow for the gas sensing data collection and analysis.

After the acquisition of raw data, preprocessing steps such as- noise filtering, normalization were performed on it. The gas response analysis is mainly performed here using two approaches: unsupervised and supervised classification. Principal component analysis is an unsupervised method of feature extraction and identification. The basic idea of PCA is to transform the original features into a set of new features in order of importance through a set of orthogonal vectors [9]. These new features are linear combinations of the original features and they are unrelated to each other. The features extracted from the training data utilizing PCA will be applied on test dataset for gas identification. Next, different supervised classification algorithms including decision tree, support vector machine, naive Bayes (kernel) and k-nearest neighbor were optimized using the training dataset. Herein, a 5-fold cross validation (CV) approach was utilized to avoid the overfitting in the training data. Finally, classification accuracy and overall performance of all the considered classifiers will be evaluated and compared to find out the optimal algorithm for precise gas identification.

III. Results and Discussion

A. Gas Sensing Properties

All the singular gas sensing data was collected in dry air under UV light at room temperature (20 °C). Before the target gas exposure, the sensor array was kept under dry air for 10 minutes. This allowed to stabilize each sensor within the array and provided us the no gas responses of all the sensors. The sample raw data response profile is given in Figure S1 in the Supporting Information section. Figures 3-4 show the responses and corresponding fitting lines of each sensor within the array toward all the target gases at various concentrations. Each response value plotted is the average response of three consecutive gas exposure responses at the same concentration for a certain analyte gas. The concentration axis is represented in a logarithmic scale to accommodate different target concentration ranges. The ppm ranges tested for NO_2, ethanol, SO_2, H_2 and O_2 are from 0.1 to 500, 50 to 5000, 0.1 to 500, 0.1 to 100 and 10000 to 400000, respectively. Then, the array sensors were exposed to different relative humidity levels, such as- 5%, 10%, 30%, 50%, 70% and 90% at room temperature (20 °C). The humidity responses are shown in Figure S2 and S3 in Supporting Information. It is clearly seen that all the individual TiO_2 and ZnO based sensors exhibited high sensitivity and excellent sensing linearity to almost all target gases. This reveals the well-known cross-sensitive behavior of metal/metal-oxides toward environmental gases.

It was found from our previous research that GaN/TiO_2 sensor response is slightly enhanced with increasing humidity and got almost constant at high humid conditions. Also, a diminishing response increase was seen at higher operating temperatures. This trend was observed for GaN/ZnO sensor as well. It is observed that sensor baseline resistances are mainly altered due to high humidity for the fabricated sensor devices. The proposed data analysis technique is based on absolute response magnitude only, no baseline information is required here. Table 1 summarizes the fitting equations and regression coefficients from the response vs concentration plots. Also, average response/recovery times for each material and gas have been presented here.

The selectivity issue of these metal/metal-oxides can be well addressed by employing sensor array technique instead of a single sensor [10]. Each gas leaves a unique response

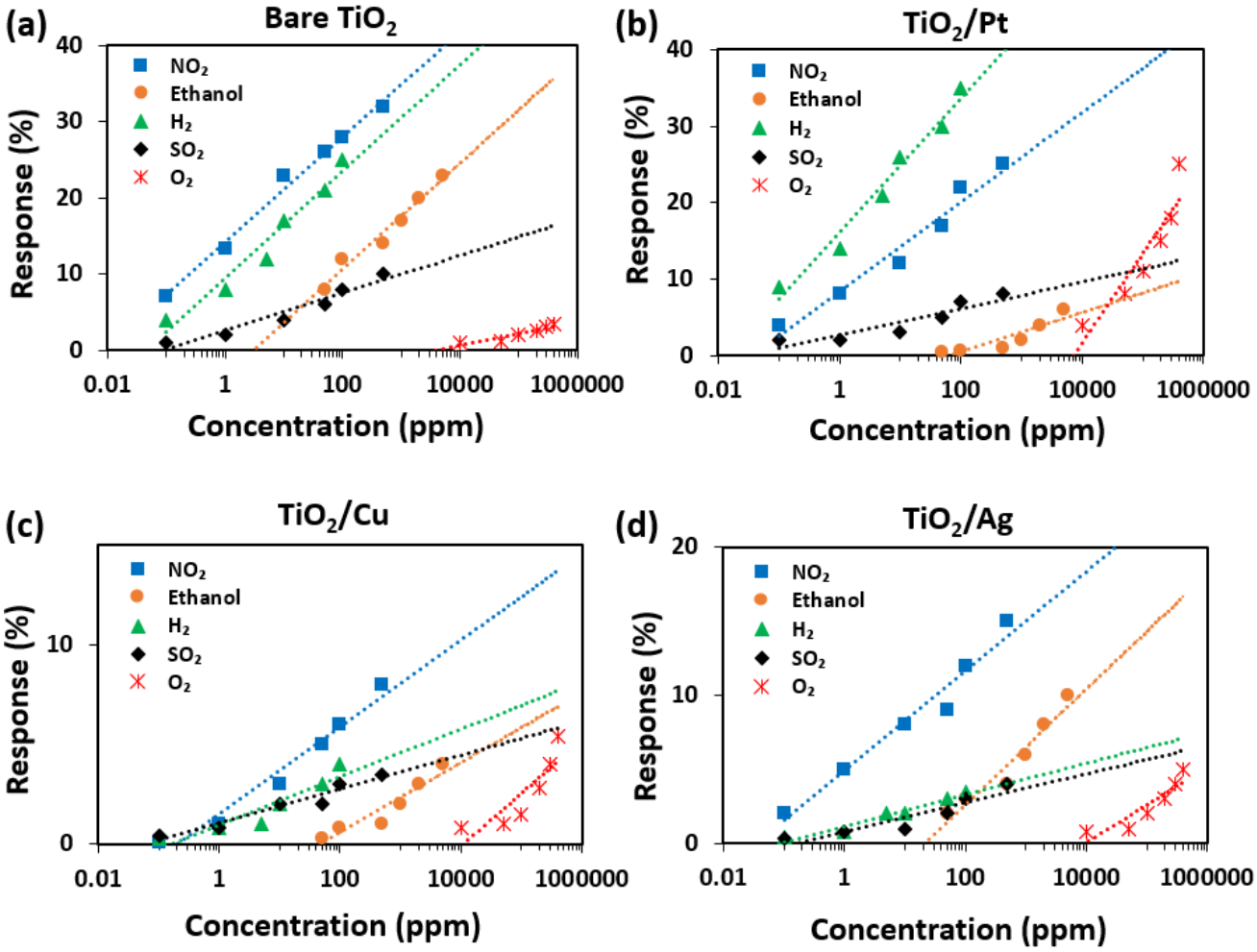

Fig. 3. Response fitting lines of (a) bare TiO_2, (b) TiO_2/Pt, (c) TiO_2/Cu, and (d) TiO_2/Ag for varying concentrations of NO_2, ethanol, SO_2, H_2 and O_2 gases in dry air under UV light at room temperature (20 °C).

footprint across the sensor array. This obtained footprint can be further analyzed by principal component analysis (PCA) and machine learning algorithms for precise identification of a target gas.

B. Principal Component Analysis on Array Response

Principal component analysis (PCA) is a mathematical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated attributes into a set of values of uncorrelated attributes called principal components [11]. In our case, all eight sensor-responses from the array were the correlated attributes which had been transformed into a set of uncorrelated principal components. Also, the redundancy of the correlated metal/metal-oxide responses from the array was resolved by smaller number of principal components that accounted for most of the variance in the observed attributes. The first principal component (PC 1) captures the maximum amount of variance possible in the original data set. On each gas exposure at a test concentration, eight response magnitudes from sensor array were used as input parameters in PCA analyses. For the target environmental gases such as- NO_2, ethanol, SO_2, H_2, O_2 and H_2O, we collected gas responses for 6 different concentrations and repeated the measurements for three times. The input PCA dataset was a 120 x 8 matrix in which 60% had been used as training set and 40% was applied as test set. The component analyses comprised a variance threshold of 98%. Since different input features have different scale, each has been normalized with its statistical mean and standard deviation. Figure 5(a) shows resulting PCA score plot where each gas clusters together displaying clear separations among them. The relative contribution of the principal components- PC 1, PC 2 an PC 3 were obtained as 64.38%, 18.53% and 12.19%, respectively, comprising 95.1% of the total variance. Rest of the insignificant components captured the residual variance. Though 3-4 sensors are enough for separation, we have taken an array of 8 sensors for building up a strong response pattern and robust classification model to accommodate large calibration variations.

By investigating the eigenvectors (loadings) of the principal components, it is possible to find out which sensor of the sensor array is best suitable for the discrimination of the target gases. These component loadings in PCA are the correlation coefficients between the principal components and sensors within the array as shown Figure 5(b). Since the first principal

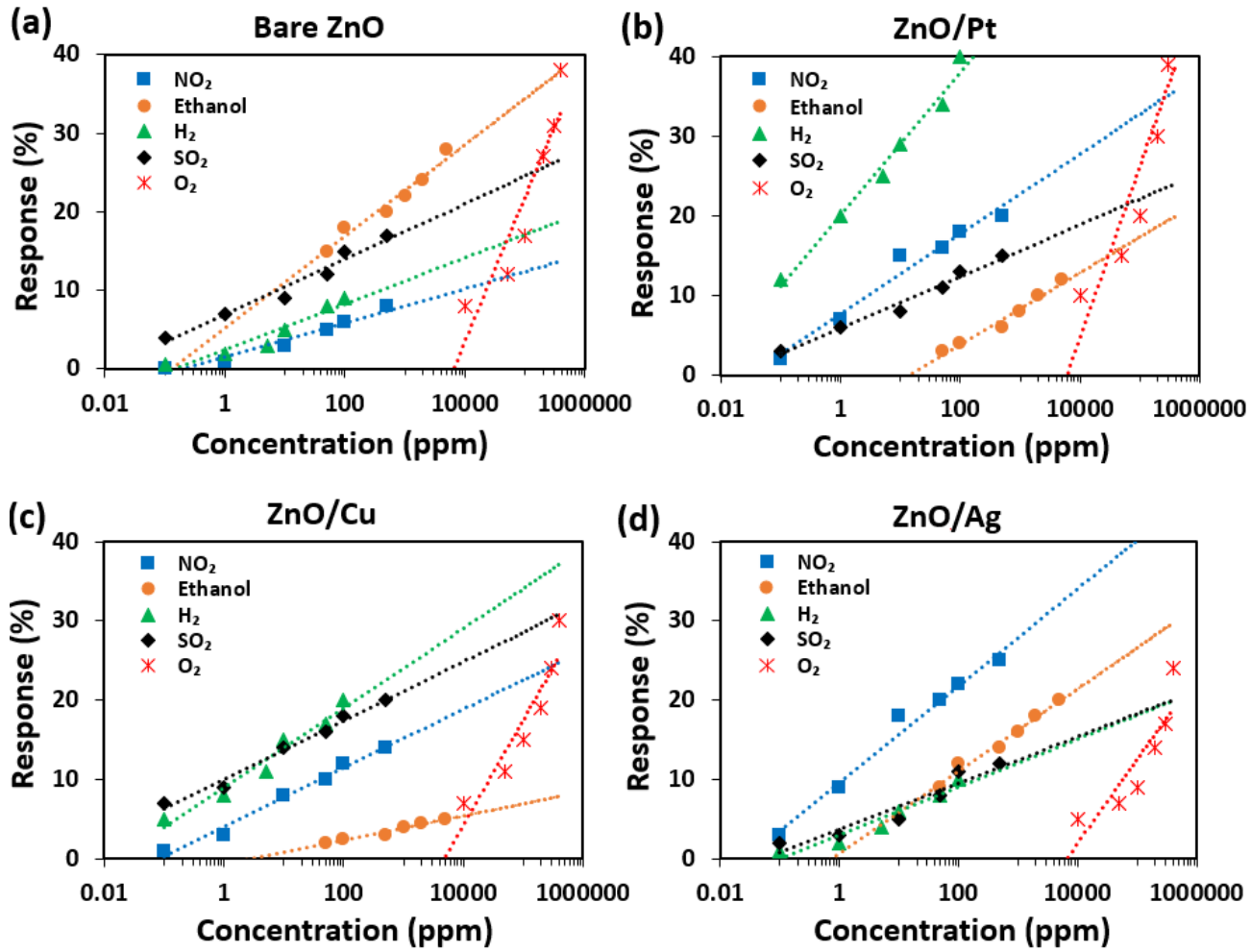

Fig. 4. Response fitting lines of (a) bare ZnO, (b) ZnO/Pt, (c) ZnO/Cu and (d) ZnO/Ag for varying concentrations of NO_2, ethanol, SO_2, H_2 and O_2 gases in dry air under UV light at room temperature (20 °C).

TABLE I
FITTING EQUATION PARAMETERS, REGRESSION COEFFICIENTS AND AVERAGE RESPONSE/RECOVERY TIMES OF SENSOR RESPONSES IN THE ARRAY

Gas	Bare TiO_2	TiO_2-Pt	TiO_2-Cu	TiO_2-Ag	Bare ZnO	ZnO-Pt	ZnO-Cu	ZnO-Ag
NO_2	3.0ln(x)+14 0.988 140s/160s	2.5ln(x)+8.4 0.959 130s/140s	.95ln(x)+1.5 0.961 160s/200s	1.4ln(x)+5 0.962 135s/140s	.95ln(x)+1.5 0.961 140s/160s	2.2ln(x)+7.6 0.968 138s/150s	1.6ln(x)+4 0.984 140s/150s	2.6ln(x)+9.6 0.980 142s/170s
Ethanol	3.0ln(x)-3.5 0.965 155s/180s	1.1ln(x)-4.7 0.802 162s/170s	.76ln(x)+2.9 0.988 145s/180s	1.7ln(x)-5.1 0.932 155s/178s	2.5ln(x)+5 0.958 160s/180s	1.9ln(x)-5.1 0.971 150s/170s	.66ln(x)-.64 0.964 165s/190s	2.2ln(x)+.64 0.978 145s/178s
SO_2	1.1ln(x)+2.5 0.940 180s/200s	0.7ln(x)+2.6 0.847 170s/195s	.37ln(x)+1 0.938 205s/220s	.42ln(x)+.82 0.860 170s/200s	1.5ln(x)+6.9 0.960 185s/210s	1.4ln(x)+5.9 0.979 160s/190s	1.6ln(x)+10 0.985 190s/220s	1.3ln(x)+3.7 0.915 175s/202s
H_2	3.0ln(x)+9.3 0.959 132s/150s	3.8ln(x)+16 0.973 145s/160s	.52ln(x)+.97 0.863 155s/180s	.46ln(x)+1.2 0.954 140s/155s	1.3ln(x)+2.4 0.923 148s/163s	3.9ln(x)+20 0.983 125s/140s	2.1ln(x)+8.9 0.959 150s/170s	1.3ln(x)+2.9 0.931 144s/170s
O_2	0.7ln(x)-5.6 0.875 138s/175s	5.1ln(x)-45 0.858 130s/160s	1.2ln(x)-10.7 0.739 150s/200s	1.1ln(x)-10 0.819 145s/185s	7.9ln(x)-69 0.870 155s/195s	9.3ln(x)-81 0.857 132s/187s	5.7ln(x)-48 0.869 160s/210s	4.6ln(x)-40 0.776 158s/192s

component carries a large part of the total variance, all the sensors equally contribute the loadings of the PC 1.

In order to evaluate the sensor array performance in a gas mixture conditions, we generated two different mixtures from our target gases which are NO_2, SO_2, O_2 and H_2O as mixture-1 and ethanol, H_2, O_2 and H_2O as mixture-2. Within each mixture, O_2 and H_2O concentrations were kept fixed at 20000 ppm and 50% RH, respectively, whereas other two gas concentrations had been varied as similar as the singular gas case. Therefore, we produced total 36 (6 × 6)

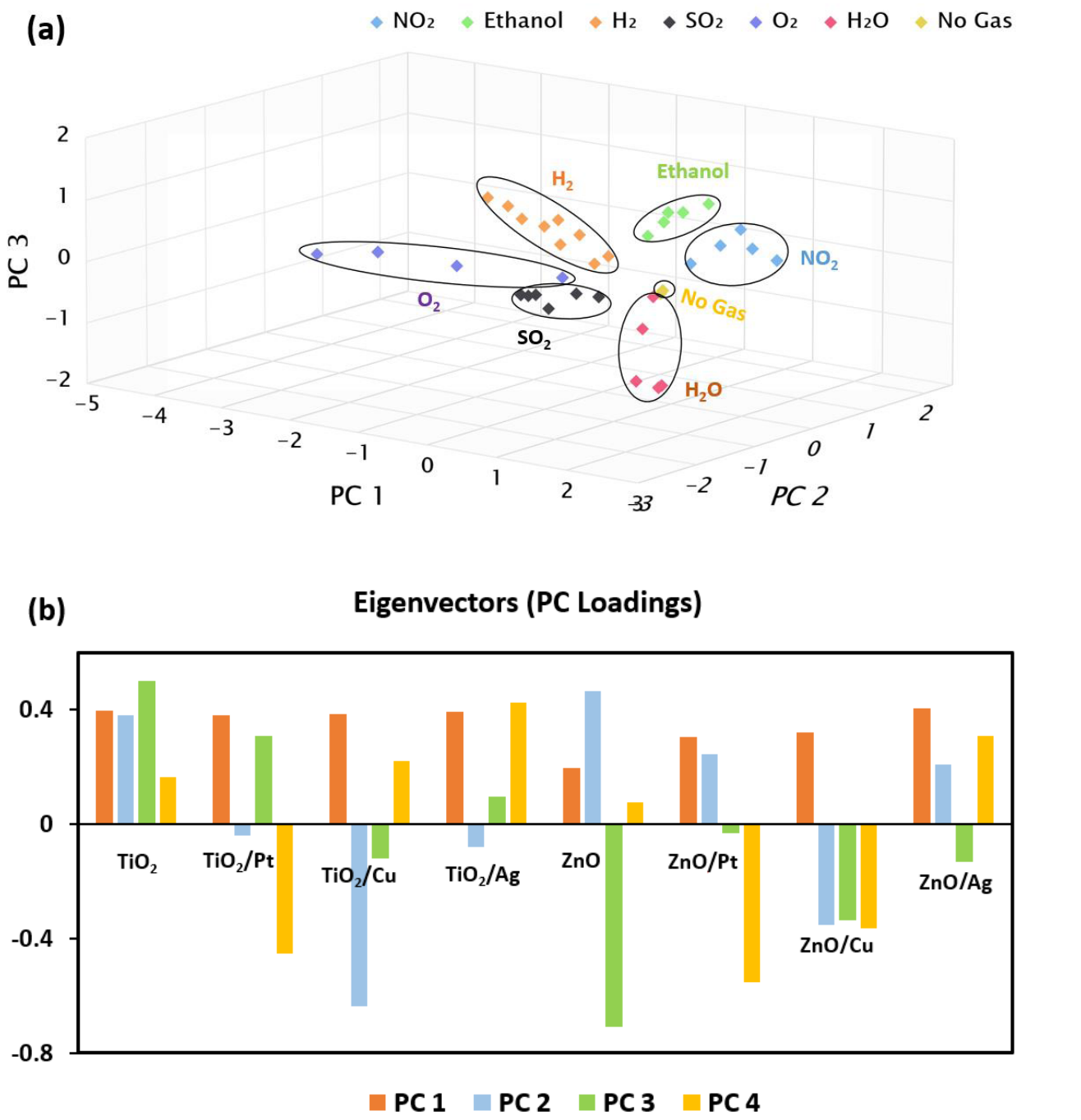

Fig. 5. (a) PCA score plot for varying concentrations of NO_2, ethanol, SO_2, H_2, $O_2$and H_2O, which includes up to 95.1% of the total variance. (b) Eigenvectors (loadings) of the first four principal components.

different concentration combinations for each mixture. These gas mixture responses obtained from the sensor array was used to build a new 72×8 (for two runs) training dataset. Based on this gas mixture training data, new PCA model was generated. These gas mixture PCA models were tested with our previous test dataset for singular gas case. The resulting PCA score plots are shown in Figure 6. It is seen that reference individual gases are still identified clearly based on the gas mixture model. This is a confirmation that the reference singular-gas dataset can be used to identify the target gases both in isolated and mixed condition.

C. Machine Learning Algorithms on Array Response

In recent years, supervised classification approaches had been applied in sensor array data to classify the analytes [12]. We have optimized and employed four different classifying algorithms on our sensor array dataset to screen out the optimal classifier for precise identification of the target gases in singular and mixed condition. Firstly, decision tree (DT) has been applied which is a collection of nodes intended to create a decision on values affiliated to a class. Taking the important DT parameters such as information gain, Gini index, maximal tree depth and minimal

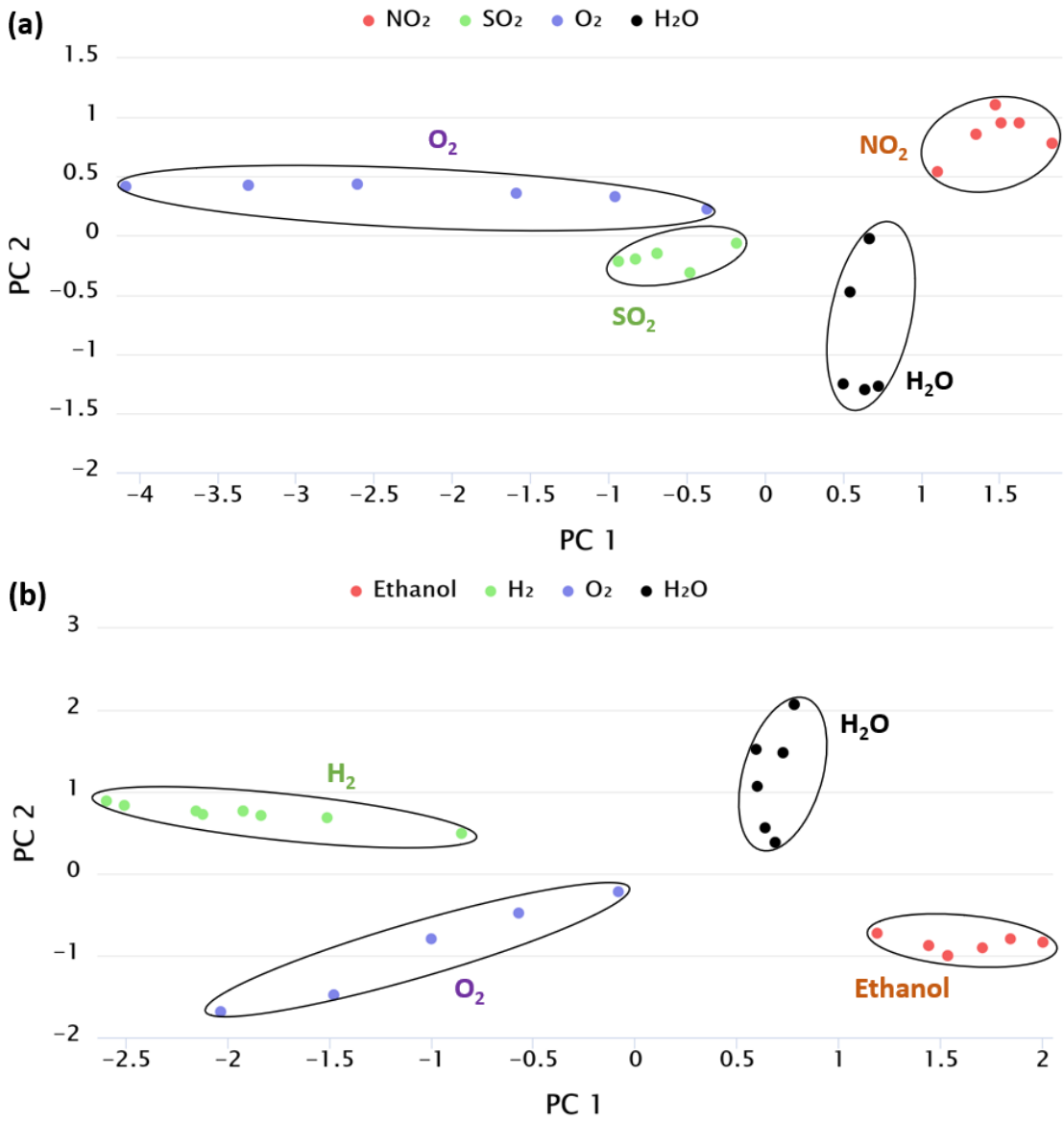

Fig. 6. PCA score plot for (a) gas mixture-1 and (b) gas mixture-2, which include up to 96.5% and 98% of the total variance, respectively.

TABLE II
SUMMARY OF THE OPTIMIZED PARAMETERS FOR THE FOUR CONSIDERED CLASSIFICATION ALGORITHMS.

Decision Tree (DT)	Support Vector Machine (SVM)	Naive Bayes (NB)	k-Nearest Neighbor (k-NN)
criterion= information gain maximal tree depth= 9 minimal leaf size= 1	kernel type= linear kernel cache= 200 C= 0.5 convergence epsilon n= 0.1	estimation mode= greedy minimum bandwidth= 0.01 number of kernels= 11	k-value= 1 kernel type= linear divergence= generalized

leaf size as variables, we found out the optimized values of these parameters for maximum classification accuracy. Next, we employed support vector machine (SVM) classifier that constructs a set of hyperplanes in a high-dimensional space for class separation. Here, parameters like kernel type, kernel cache, C and convergence epsilon were optimized.

Then, comparatively simpler Naive Bayes (kernel) algorithm was used which is a probabilistic classifier based on Bayes' theorem with strong (naive) independence assumptions. Estimation mode, minimum bandwidth and number of kernels were varied within the standard algorithm. Lastly, k-Nearest Neighbor (k-NN) algorithm was applied on our array dataset. It is based on comparing an unknown example with the

(a)	true NO_2	true Ethanol	true H_2	true SO_2	true O_2	true H_2O
pred. NO_2	8	0	0	0	0	0
pred. Ethanol	0	10	0	0	0	0
pred. H_2	0	0	11	0	0	0
pred. SO_2	0	0	0	10	1	0
pred. O_2	0	0	0	0	5	0
pred. H_2O	0	0	0	0	0	5

(b)	true NO_2	true Ethanol	true H_2	true SO_2	true O_2	true H_2O
pred. NO_2	8	0	0	0	0	0
pred. Ethanol	0	10	0	0	0	0
pred. H_2	0	0	11	0	0	0
pred. SO_2	0	0	0	10	0	0
pred. O_2	0	0	0	0	6	0
pred. H_2O	0	0	0	0	0	5

(c)	true NO_2	true Ethanol	true H_2	true SO_2	true O_2	true H_2O
pred. NO_2	8	0	0	0	0	0
pred. Ethanol	0	10	0	0	0	0
pred. H_2	0	0	11	0	0	0
pred. SO_2	0	0	0	10	0	0
pred. O_2	0	0	0	0	6	0
pred. H_2O	0	0	0	0	0	5

(d)	true NO_2	true Ethanol	true H_2	true SO_2	true O_2	true H_2O
pred. NO_2	8	0	0	0	0	0
pred. Ethanol	0	10	0	0	0	0
pred. H_2	0	0	11	0	0	0
pred. SO_2	0	0	0	9	1	0
pred. O_2	0	0	0	1	5	0
pred. H_2O	0	0	0	0	0	5

Fig. 7. The confusion matrix of (a) Decision Tree classifier, (b) Support Vector Machine (SVM) classifier, (c) Naive Bayes (kernel) classifier, and (d) k-Nearest Neighbor (k-NN) classifier.

k training examples which are the nearest neighbors of the unknown example. The accuracy has been maximized here by optimizing the k-value, kernel type and divergence parameters. The array sensor responses of training data were used to model these algorithms, and then gas types from the test data were qualitatively identified by the models. In order to adapt naive Bayes and support vector machine (SVM) algorithms for multiclass discrimination problem, regression learning algorithm has been utilized in a subprocess that generates regression learner model. Here, the binary NB and SVM classifiers build multi-class classification model using the developed regression model. Table 2 summarizes the parameters optimized for building these four considered classification algorithms.

Figure 7 shows the confusion matrices for the four classifiers. The values on the diagonal are the correctly identified class of each category. Classification accuracy (η) for each classifier has been calculated which is defined by: $\eta =$ (sum of diagonal values) / (total classification data). It is found that both SVM and NB exhibited 100% accuracy whereas DT and k-NN attained an accuracy of 98% and 96%, respectively. Furthermore, DT algorithm becomes less accurate and tough to implement when number of decisions in a tree increases. The accuracy of the *k*-NN algorithm can be severely degraded by the presence of noisy or irrelevant features. On the other hand, SVM has the advantage of higher efficiency for correct classification of the future data without over-fitting. Again, NB classifier offers faster convergence and simpler implementation. Therefore, depending on the application, both SVM and NB are suggested to be the best suitable algorithms for precise identification of our target gases and their mixtures.

IV. Conclusion

Metal/metal-oxide based gas detection suffers from inevitable cross-sensitivity against the interferant gases. Improving the gas discrimination by using array of sensors having different characteristics has been considered as a potential solution to this problem. In this paper, we report the results of sensor array having eight different metal/metal-oxide functionalized GaN nanowires made by industry standard

top- down fabrication approach. For the detection of NO_2, ethanol, SO_2, H_2, H_2O and O_2 gases, receptor layer combinations such as- Pt, Cu and Ag decorated TiO_2 and ZnO have been obtained from our prior DFT simulation study. All the gas response data were collected for single and mixture of gases under UV light at room temperature. PCA study was performed on the array response and results show that gas clusters exhibit clear separations among them. Next, machine learning algorithms such as- DT, SVM, NB (kernel) and k-NN were trained and optimized using their important parameters to screen out the optimal algorithm. Results indicate that SVM and NB classifier models exhibited full classification accuracy on our dataset. In addition, the developed array device consumes very low power because of UV assisted sensing as compared to commercially available metal-oxide sensors.

Acknowledgment

The sensor array was fabricated in the Nanofab of the NIST Center for Nanoscale Science and Technology. Gas sensing measurements were conducted at N5 Sensors, Inc.

Conflicts of Interest

There are no conflicts of interest to declare.

References

[1] *Occupational Safety and Health Administration (OSHA) (2017) Air Contaminants*. Accessed: Apr. 4, 2018. [Online]. Available: https://www.osha.gov/dsg/annotated-pels/tablez-1.html

[2] M. Khan, M. Rao, and Q. Li, "Recent advances in electrochemical sensors for detecting toxic gases: NO_2, SO_2 and H_2S," *Sensors*, vol. 19, no. 4, p. 905, Feb. 2019.

[3] J. Ree, Y. H. Kim, and H. K. Shin, "Dynamics of gas-surface interactions: Reaction of atomic oxygen with chemisorbed hydrogen on Tungsten," *J. Phys. Chem. A*, vol. 101, no. 25, pp. 4523–4534, Jun. 1997.

[4] Y.-F. Sun *et al.*, "Metal oxide nanostructures and their gas sensing properties: A review," *Sensors*, vol. 12, no. 3, pp. 2610–2631, Feb. 2012.

[5] N. Akiyama, "A sensor array based on trigonal-selenium nanowires for the detection of gas mixtures," *Sens. Actuators B, Chem.*, vol. 223, pp. 131–137, Feb. 2016.

[6] M. A. H. Khan, B. Thomson, R. Debnath, A. Rani, A. Motayed, and M. V. Rao, "Reliable anatase-titania nanoclusters functionalized GaN sensor devices for UV assisted NO_2 gas-sensing in ppb level," *Nanotechnology*, vol. 31, no. 15, Dec. 2019, Art. no. 155504.

[7] M. A. H. Khan, B. Thomson, J. Yu, R. Debnath, A. Motayed, and R. V. Mulpuri, "Scalable metal oxide functionalized GaN nanowire for precise SO_2 detection: Experimental results and density functional theory modeling," *Sens. Actuators B, Chem.*, submitted for publication.

[8] M. A. H. Khan, B. Thomson, A. Motayed, Q. Li, and R. V. Mulpuri, "Functionalization of GaN chemical sensors with metal oxides," *IEEE Sensors J.*, submitted for publication.

[9] S. X. Wu, H.-T. Wai, L. Li, and A. Scaglione, "A review of distributed algorithms for principal component analysis," *Proc. IEEE*, vol. 106, no. 8, pp. 1321–1340, Aug. 2018.

[10] G. Magna *et al.*, "Conductive photo-activated porphyrin-ZnO nanostructured gas sensor array," *Sensors*, vol. 17, no. 4, p. 747, Apr. 2017.

[11] J. Lever, M. Krzywinski, and N. Altman, "Principal component analysis," *Nature Methods*, vol. 14, pp. 641–642, Jun. 2017.

[12] S. Fan, Z. Li, K. Xia, and D. Hao, "Quantitative and qualitative analysis of multicomponent gas using sensor array," *Sensors*, vol. 19, no. 18, p. 3917, Sep. 2019.

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