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MACHINE LEARNING ASSISTED OPTIMIZATION OF NANOSTRUCTURED CHALCOGENIDES FOR RAPID AND SELECTIVE MULTI-GAS SENSING INTEGRATED WITH THERMOELECTRIC DEVICES

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ABSTRACT

The increased need of fast, selective, and energy-efficient gas sensing technologies has intensified the search of the low-dimensional nanostructured materials and data-driven optimization approaches. The traditional design of gas sensors is based on the trial-and-error strategies, which are not scalable, and materials discovery is slow. Here, machine learning (ML) has become a disruptive technology of predicting sensing performance, material property optimization, and discrimination of intelligent gases. This review is a critical analysis of the combination of ML methods with nanostructured chalcogenide materials, namely, SnSe 2, WSe 2, Bi 2S 3 and Bi 2Se 3 as biosensors to be used in conjunction with thermoelectric devices. These materials have a great potential to be utilized as high-sensitivity sensing platforms because of their unique electronic structures, high surface-volume ratios, and tunable defect chemistry that offer better adsorption sites, and enhanced charge transfer. Artificial neural networks, support vector machines, and ensemble learning models have been demonstrated to possess a great potential in the extraction of features, gas classification, predicting the responses, and optimization of operating temperatures. Moreover, the addition of thermoelectric effects allows self-powered sensing and a better stability of the signal, and can be used as a step forward towards autonomous sensor systems. Although these have been made, there are still issues of poor standardized datasets, overfitting with small experimental datasets, and interpretable ML frameworks to understand mechanisms. Innovation areas like transfer learning, digital twins and explainable artificial intelligence are likely to expedite the process of materials discovery and sensor optimization. The review gives an insightful thematic overview of the current developments, the most important gaps in the research, and the perspectives of future research on the use of ML in the design of self-powered, high-performance multi-gas sensory platforms.

KEYWORDS: Machine Learning, Nanostructured Chalcogenides, Multi-Gas Sensing, Thermoelectric Sensors, Selectivity Optimization, $SnSe_2$, WSe_2, Bi_2S_3, Bi_2Se_3

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Research Paper

1. INTRODUCTION

Gaseous species detection and monitoring is important in the environmental protection of the surroundings, industrial health and diagnostics of the medical profession. Existing toxic and inflammable gases like NO 2, NH 3, CO, H2S and volatile organic compounds (VOCs) are very dangerous to human health and manufacturing processes and therefore, advanced and sensitive gas sensing devices are required. Real-time monitoring of air pollutants is needed in environmental applications in order to lower climate-related and urban air quality challenges. This has necessitated rapid detection systems in industrial environments to bar leakages and explosions whereas in the medical field breath analysis has come as a non-invasive diagnosis of medical conditions, including diabetes, asthma, and lung cancer. These various applications require a sensor not only of the highest level of sensitivity but also that which can differentiate between a variety of gases within varying operating conditions.

Traditional gas sensors mostly metal oxide semiconductor transduced gas sensors have proven to be highly sensitive, but have poor selectivity, high operating temperatures, slow response and recovery times and are very power hungry. This problem is further complicated in a multi-gas situation, where the cross-sensitivity and signal overlap prevents the discrimination of the gases accurately. Consequently, there is the increasing demand of fast, selective, and low power sensing platforms that can be used under ambient conditions with high performance.

Next-generation gas sensors Low-dimensional nanostructured materials have come up as good candidates because of their properties of unique physicochemical properties. Layered chalcogenides with two dimensions, like SnSe 2 and WSe 2, and one-dimensional and nanostructured Bi 2 S 3 and Bi 2 Se 3 have high ratios of surface to volume, tunable bandgaps and rich active sites to gas adsorption. These properties improve charge transfer interactions between the sensing material and target gas molecules, and thus, the dynamics of sensitivities and responses are better. Also, the selective detection of gases by these nanomaterials can be further enhanced through defect engineering, heterostructure formation and surface functionalization of these nanomaterials to tune the adsorption energies and electronic transport pathways.

The most recent approach to overcome the power consumption problem in gas sensing is the implementation of thermoelectric effects in sensing platforms. Using the Seebeck effect, thermoelectric materials can produce an electrical voltage as a result of a temperature gradient to allow the creation of self-powered gas sensors. The Chalcogenide materials, SnSe 2 and Bi 2 Se 3, have been found to have good thermoelectric characteristics that include high Seebeck coefficients and low thermal conductivity and thus would be suitable to dual function sensing and energy harvesting systems. The thermoelectric functionality paired with gas sensing is coupled with a reduction in the amount of external power needed to maintain this operation, as well as stability of the signal and the ability to work in remote or wearable applications.

In spite of the major progress in producing nanomaterials and devices, the identification and optimization of high-performance sensing materials are widely based on the empirical and time-consuming trial-and-error techniques. The large parameter space of material composition, morphology, defect density, operating temperature and gas concentration presents a difficult problem of systematic optimization. In efficiency to determine optimal material-gas combinations and the ability to discover widely nonlinear interrelationships of sensor behavior, traditional experimental workflows are inefficient.

Machine learning (ML) has become an effective instrument in this regard to speed up the discovery of materials and sensor optimization. ML algorithms will be able to process data of large experiments and computations and determine patterns that are not visible, forecast sensing reactions, and streamline material characteristics. Artificial neural networks, support vector machines, random forests and deep learning models have been successfully utilized in gas classification, feature extraction via sensor arrays, response prediction and operating temperature optimization. ML design enables the data-driven design to reduce the amount of work done in experiments, make the process more selective in multi-gas environment, and real-time adaptive sensing.

More so, combination of ML with nanostructured thermoelectric gas sensors allows intelligent sensing systems which can self-calibrate, compensate drift and work autonomously. Examples that these systems are applicable to include Internet of Things (IoT)-based environmental monitoring and wearable healthcare devices. Nevertheless, there are still a number of issues such as the inadequate access to standardized datasets, overfitting of a model at any small sample regime, non-interpretability of complex ML models, and the necessity to provide scalable synthesis of nanostructured materials.

This review aims at a critical analysis and evaluation of the recent achievements in machine learning-assisted optimization of nanostructured chalcogenides, namely $SnSe_2$, WSe_2, Bi_2S_3, and Bi_2Se_3, to obtain fast and selective multi-gases sensing with thermoelectric sensors. The review will (i) provide an overview of the basic gas sensing principles and thermoelectric principles applicable to these materials, (ii) discuss the effects of nanostructuring on sensing, (iii) discuss the use of ML in optimization and gas selectivity of the sensors, (iv) discuss present-day challenges and gaps in research and (v) provide future perspectives of the multi-gas sensing systems based on the self-powered nanostructured sensor designs.

2. FUNDAMENTALS OF GAS SENSING AND THERMOELECTRIC NANOMATERIALS

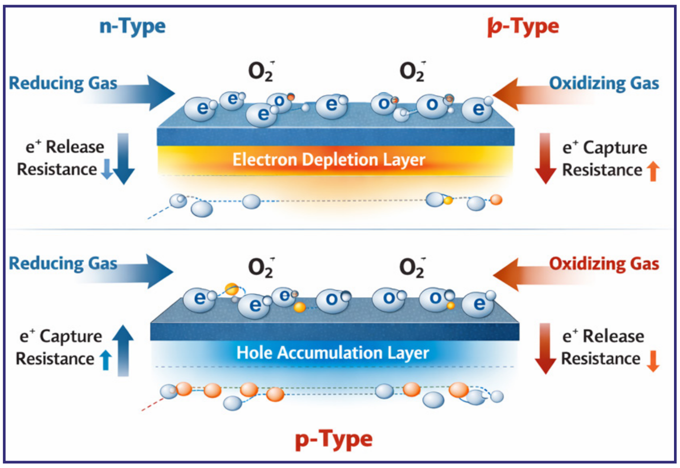
2.1 Gas Sensing Mechanisms

The process of gas sensing in nanostructured semiconducting materials is majorly controlled by physicochemical interactions at the surfaces that control electrical transport properties. The most commonly used sensing principles include chemoresistive mechanism which is the simplest, high sensitivity and compatible with low-dimensional material. Chemoresistive sensors detect the adsorption of gases to the surface of the material, which leads to a change in electrical resistance. This variation is a result of the modulation of charge carrier concentration occasioned by surfaces reaction of the sensing substance and target gas species.

The surface adsorption and desorption processes form the major factor in sensor response. Under ambient conditions, oxygen molecules are usually adsorbed to the surface of the n-type semiconducting materials in the form of ionized species (O_2^-, O^- or O^{2-}) extracting electrons in the conduction band to form a depletion layer. Upon a reducing gas like NH_3 or H_2S interacting with the surface, this gas reacts with the adsorbed oxygen ions releasing trapped electrons to the conduction band and reducing the sensor resistance. On the other hand, oxidizing gases like NO_2 also deprive the electrons and this hikes resistance. In p-type material the resistance change occurs in the inverse direction as the conduction is based on holes.

The strength and direction of sensor response in relation to adsorbed gas molecules is dictated by charge transfer between the sensing material and the gas molecules. Low-dimensional chalcogenides ($SnSe_2$, WSe_2, Bi_2S_3, and Bi_2Se_3) have high surface to volume ratios and tunable electronic bands, and therefore are capable of facilitation of charge transfer and increased sensitivity. The defect sites, edge states and heterostructure interfaces are the active adsorption centers that enhance the interaction strength with special gas molecules and provide selective detectability. Response and recovery properties are also determined by kinetics of adsorption-desorption processes, and this aspect is important to real-time sensing applications.

Figurative illustration of chemoresistive gas sensing mechanism of oxygen adsorption, electron depletion layer, and resistance change of n-type and p-type chalcogenide nanostructures under different gases reducing and oxidizing conditions.



5.2 Thermoelectric Effect in Sensing Platforms

The incorporation of thermoelectric into gas sensing stationary creates a self-sufficient route of power generation. The effect that can be described as the thermoelectric effect, specifically the Seebeck effect, is the occurrence of an electrical voltage across a substance when a temperature difference is created between its opposite extremes. The size of the voltage produced is proportional to Seebeck coefficient and temperature difference applied. $SnSe_2$ and Bi_2Se_3 are examples of chalcogenide materials, which have high Seebeck coefficients, low thermal conductivity, and good electrical transport properties, and go into use in thermoelectric sensing applications.

Gas adsorption changes the local carrier concentration as well as scattering processes in thermoelectric gas sensors, which then change the Seebeck coefficient and electrical conductivity. This two mode modulation allows gas sensing by the thermoelectric variation of voltage and does not require constant external power source. This type of self-powered sensing is especially beneficial to remote sensing, wearable computing, and environmental sensing systems based on Internet of Things (IoT). Thus, the thermoelectric coupling can enhance the stability of signals providing stability, reducing the thermal noise, and allowing simultaneous harvesting and sensing.

5.3 Performance Parameters

The gas sensors are tested in relation to various parameters that are considered as the most important such as the sensitivity, the selectivity, the response and recovery time, and the operating temperature. The sensitivity degree of the electrical or thermoelectric signal upon exposure to a target gas is defined as such, the sensitivity depends on the surface area, adsorption energy, and efficiency of charge transfer. Highly sensitive nanostructured materials are usually high surface activity, which is characterized by a high number of interaction sites.

Selectivity is the property of a sensor to be selective to a given gas under the influence of interfering species. High selectivity is also a significant problem in chemoresistive sensing and frequently necessitates functionalization of material, heterostructure or pattern recognition algorithms coupled with sensor arrays. The extraction of features with the help of machine learning has become a potential solution to selectivity constraints in multi-gas settings.

Response time This is the time needed by the sensor to attain a desired percentage (usually 90 percent) of the maximum signal change when exposed to a gas and recovery time is the time needed to regain the baseline after the gas has been removed. These parameters are controlled by adsorption desorption kinetics, diffusion, and working temperature. Smaller operating temperatures are preferred in energy efficient sensing, but they tend to slow down reaction kinetics and require catalytic dopants, light activation or thermoelectric aids to preserve the fast response nature.

Altogether, a combination of surface chemistry, electronic transport, and thermoelectric properties defines the sensing properties of nanostructured chalcogenide materials, which can serve as a basis of machine learning-aided optimization of high-performance multi-gas sensors.

6. NANOSTRUCTURED MATERIALS FOR MULTI-GAS SENSING

The nanostructures with low dimension chalcogenide have been of significant interest in multi-gas sensing as they have tunable electronic properties, high specific surface area and good surface adsorption ability. SnSe 2, WSe 2, Bi 2S 3, and Bi 2Se 3 have layered or quasi-one-dimensional structures, which offer large quantities of active sites on which to interact with gases and effective charge conduction routes. Their band architecture, defect properties and thermoelectric properties also facilitate selective and fast sensing especially when prepared at a nanoscale.

6.1 $SnSe_2$ Nanostructures

Grind has a hexagonal CdI 2 -type crystal structure, is a layered metal chalcogenide, and has an indirect bandgap of about 1.0-1.3 eV. The inter-layer van der Waals force is weak and the adjacent layers can be exfoliated easily into few-layers or nanosheets to obtain a high surface-to-volume ratio. This structural advantage increases the adsorption of gases as well as efficient charge transfer, between the adsorbed molecules and the conduction band.

SnSe 2 nanostructures are highly sensitive to gases of oxidation like NO 2 and gases of reduction like NH 3 and H 2 S. The principle of controlling the sensing mechanism is the modulation of the electron concentration in the n type semiconductor by the surface adsorption process. Morphology errors, like selenium defects, in the defect engineering, put the localized states in the form of active adsorption centers, enhancing the magnitude of response and reducing the operating temperature. Moreover, it has been demonstrated that heterostructure formation with metal oxides or metal nanoparticles of noble metals helps to increase selectivity and decrease response time through catalytic reactions on the surface.

6.2 WSe_2 Nanostructures

WSe 2 is a two-dimensional transition metal dichalcogenide with a layered structure, which has a thickness dependent bandgap switching between indirect in bulk to direct in monolayer geometry. Its mobile carrier, selectable electronic characteristics, and mechanical dexterity render it to be useful in low-temperature gas sensing.

WSe 2 defect density, edge sites and surface functionalization are all known to have a pronounced effect on the sensing performance of WSe 2. Active adsorption sites that facilitate interaction with gas molecules (NO 2, NH 3 and VOCs) are selenium vacancies and grain boundaries. Also, WSe 2 p-type conduction behavior allows complementary sensing properties relative to n-type media, which is useful in sensor array designs with the objective of multi-gas discrimination.

The separation of the charge and the enhancement of the sensing signal are achieved by functionalization with nano-particles of the metal or by creating products of heterojunctions with n-type semiconductors. There have also been reports of light-assisted sensing by WSe 2 in which the carriers generated by photons are able to increase adsorption desorption kinetics and decreasing the recovery time so that the device can work at room temperature.

6.3 Bi_2S_3 Nanostructures

Bi 2 S 3 is a narrow bandgap semiconductor (1.3 -1.7 eV) which usually exists in one-dimensional nanorods, nanowires and nanoflowers. These morphologies have high surface area and numerous adsorption sites that are useful in gas sensing purposes. Bi 2S 3 has an orthorhombic crystal structure that facilitates anisotropic charge transport, which allows simple carrier modulation in the presence of gases.

Bi 2S 3 nanostructures show high sensitivity to gases like NO 2, H 2 S, and ethanol when operating with rather low temperatures. Close proximity of states on the surfaces enhances charge transfer interactions, which result into high resistance variation when exposed to gases. Additional additions made to sensing performance and increasing the level of sensing include doping and composite formation with metal oxides or carbon based materials, which raises the electrical conductivity and adsorption capacity.

The other benefit of Bi 2 S 3 is that it can be used with flexible materials and is therefore applicable in wearable devices. Scalable device manufacturing is also enabled by its comparatively low manufacturing temperature, as well as, solution-producible production paths.

6.4 Bi_2Se_3 Nanostructures

Bi 2 Se 3 is a layered compound that is well known to exhibit topological insulator behavior, which has conducting surface states and an insulating bulk. It also has a small bandgap (c. 0. 3 e V), large carrier mobility, and is a good thermoelectric material as it has a large Seebeck number and low thermal conductivity. Bi 2 Se 3 is especially appealing as a thermoelectric gas sensor due to these properties.

Topological surface states increase conductivity of surfaces and allow transfer of charge quicker during gas adsorption; this leads to fast response and recovery times. At low operating temperatures Bi 2 Se 3 nanoplates and nanosheets proved to be sensitive to various gases including NO 2, NH 3, and H 2 S. The high level of interaction between thermoelectric and chemoresistive properties allows the dual-mode sensing, where the change in resistance and the variation in thermoelectric voltage both play a role in signal generation.

Defect engineering (in particular, selenium vacancies) is important in carrier concentration tuning and carrier adsorption tuning. Also, heterostructures made of Bi 2 Se 3 and metal oxides or graphene enhance selectivity and stability through increased interfacial charge transfer and decreased baseline drift.

6.5 Comparative Performance of Chalcogenide Nanostructures

The electronic structure, morphology, and defect chemistry of SnSe 2, WSe 2, Bi 2S 3, and Bi 2Se 3 determine the sensing performance. SnSe 2 and Bi 2 Se 3 have a strong n-type behaviour and thermoelectric compatibility which implies that they can be used in self-powered sensing platforms. WSe 2 offers p-type conduction as well as great flexibility, which allows complementary sensing in hybrid arrays. Bi 2 S3 has a great surface area and low temperature which is beneficial with portable devices.

Table 1: Comparative Gas Sensing Performance of Nanostructured Chalcogenides

Material	Target Gases	Typical Sensitivity*	Operating Temperature	Key Advantages
$SnSe_2$	NO_2, NH_3, H_2S	High (ppm to ppb)	Room temp – 150 °C	Layered structure, high electron mobility, defect tunability
WSe_2	NO_2, NH_3, VOCs	Moderate–High	Room temp – 120 °C	2D morphology, p-type conduction, light-assisted sensing
Bi_2S_3	NO_2, H_2S, Ethanol	High	50–200 °C	1D nanostructures, high surface area, low-cost synthesis
Bi_2Se_3	NO_2, NH_3, H_2S	High with fast response	Room temp – 100 °C	Topological surface states, thermoelectric compatibility

*Sensitivity values vary depending on morphology, doping, and device configuration.

In general, these chalcogenides nanostructures are diverse multi-gas sensing material platforms. Their complementary electronic properties allow sensor arrays to be designed with increased selectivity and their thermoelectric properties allow self-powered sensing through the development of self-powered systems. Engineering nanostructures in conjunction with machine learning aided optimization has a viable future towards developing fast, selective, and energy efficient gas detection.

7. MACHINE LEARNING IN GAS SENSOR OPTIMIZATION

The introduction of machine learning (ML) to gas sensing work has allowed to shift the focus of the research paradigm away towards empirical screening of materials and move to data-driven optimization. Gas sensors, and especially gas sensors operating based on nanostructured materials generate multidimensional data that depends on the composition of materials, morphology, temperature of operation, humidity, and concentration of the gas. These parameters are nonlinear and interdependent hence conventional analytical modeling will not be adequate to predict and optimize accurately. The machine learning algorithms offer the ability to learn more complicated relationships by using experimental and computational data, which can be used to discriminate gases, predict their performance, and design a smart sensor.

7.1 Machine Learning Techniques Used

One of the most common ML models used in gas sensing is the artificial neural networks (ANNs) because it can use nonlinear relationships between sensor responses and input features. Multilayer perceptron designs have been effective in converting resistance or thermoelectric data to gas type and concentration. ANNs are especially useful with the problem of cross-sensitivity when dealing with sensor arrays, where two or more gases have similar response patterns.

SVMs have shown excellent results in the classification of gases particularly in small and medium-sized datasets. SVMs are built to create ideal hyper planes in high dimensional feature space that allow correct separation of patterns of gas response even when there is noise. Their modeling of nonlinear sensing behavior is also improved by the use of kernel functions.

The random forest (RF) algorithms offer strong classification and regression capabilities to problems associated with gas sensing. RF being an ensemble learning technique, minimizes overfitting and enhances generalization by integrating several decision trees that have been suggested to learn various subsets of data. The most influential sensing parameters have been detected by using RF models, which helps to select features and optimize materials.

The gradient boosting systems such as XGBoost or LightGBM have high predictive accuracy because they reduce residual errors in a serial manner as the model is trained. Such models find application especially on predicting responses, optimization of operating temperatures and estimating concentrations. They are capable of dealing with heterogeneous datasets and are, therefore, suitable to combine experimental and features obtained through simulations.

Recently, the concept of convolutional neural networks (CNNs) and recurrent neural networks (RNNs) has been considered as a form of deep learning to identify patterns in dynamically changing gas sensor signals. CNNs are able to get spatial features of sensor array response maps whereas RNNs can be used to get temporal response features, such as response and recovery dynamics. With the help of such models, it is possible to identify gas in real-time and sense it adaptively in complex environments.

ML Model[D1.1]	Application in Gas Sensing	Strengths	Limitations
ANN	Gas classification, concentration prediction	Captures nonlinear behavior	Requires large dataset
SVM	Multi-gas discrimination	High accuracy in small datasets	Sensitive to kernel selection
Random Forest	Feature selection, response prediction	Reduces overfitting, interpretable	Higher computation for large data
Gradient Boosting (XGBoost/ LightGBM)	Temperature optimization, regression tasks	High predictive accuracy	Risk of overfitting if not tuned
CNN / RNN (Deep Learning)	Pattern recognition, dynamic signal analysis	Handles temporal & spatial features	Needs large labeled datasets

7.2 Applications of ML in Gas Sensing

ML is important in the extraction of features, as it is used to determine the most significant parameters can affect the performance of the sensor. Intrinsic characteristics like base resistance, response magnitude, response and recovery slopes, temperature dependence and frequency-domain characteristics can be automatically determined using raw sensor signals. Principal component analysis (PCA) used as a dimensionality reduction method and t-distributed stochastic neighbor embedding (t-SNE), are usually used as preprocessing tools to enhance the efficiency of the models and visualization.

One of the most obvious uses of ML in multi-gas sensing is gas classification. Sensors arrays made of complementary sensing material yield different response patterns to different gases. ML models are able to acquire such patterns and reach high classification accuracy, even with the presence of interfering gases, and in a different environmental condition.

The concept of selectivity enhancement is attained via pattern recognition and elimination of adsorption of individual materials based on material-specific properties of adsorption. Discrimination of gases with similar physicochemical behavior is possible by using multidimensional response signatures that are analyzed by the ML algorithms. This method excludes the use of highly selective single-material sensors by a great margin.

Response prediction and estimation of concentration are also carried out using ML models. Regression algorithms can also be used to approximate sensor output to unobservable gas concentrations, where calibration-free sensing can be used, as well as where detailed experimental measurements are unnecessary. These predictive models are of great use in optimizing a material and also in the operating conditions of the device.

Another useful use is that of optimization of operating temperature. ML algorithms have the capability of determining the optimal temperature ranges that are sensitive and consumes minimal power usage and response time. This is especially so to the case of thermoelectric gas sensors, in which temperature gradients have an effect on sensor and energy harvesting functionality.

7.3 Data Sources for ML Models

The training data determines the performance of ML models. Real world response characteristics of chemoresistive sensors or thermoelectric sensors that are obtained by measuring experimental datasets give the data of the various gas concentrations and environmental conditions. Such data usually entail resistance modification, response time, recovery time and operating temperature.

DFT-based simulation data is useful in understanding adsorption energies, a mechanism of charge transfer, density of states and the change in band structure when gases are adsorbed. The combination of DFT-derived characteristics and experimental results can be used to improve the interpretability of the model and predict the sensing performance on new material-gas regimes.

Sensor arrays produce high-dimensional measurements of cross-selective responses of a variety of materials. They are especially well-suited datasets to gas classification and pattern recognition with the help of ML. Also, given that time-series data of dynamic sensing experiments provide time-varying information, deep learning models can be used to extract time-related features and identify the gas in real-time.

7.4 ML Workflow for Materials Design

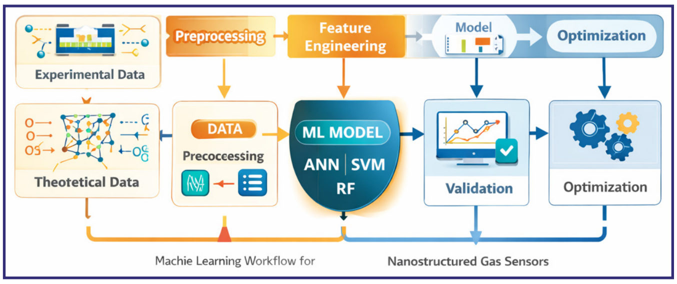
The generic workflow of the ML-based optimization of gas sensors includes numerous steps that start with the collection of experimental and simulated measurements, as well as literature databases. The data collected is subjected to preprocessing measures of normalization, noise filtering and missing values. This is followed by feature engineering that is done to obtain meaningful descriptors, such as material properties, morphological parameters, adsorption energies and electrical response measures.

The processed data is separated into training, validation, and test data to guarantee fair results of model analysis. The use of the appropriate ML algorithms depends on the problem type, e.g. classification to identify gas or regression to predict responses. Hyperparameter tuning is done to achieve better performance of the model without overfitting.

Statistical measures that are used to verify model validation include accuracy, precision, recall, F1-score of classification, and mean squared error or coefficient of determination of regression tasks. The methods of cross-validation also improve the reliability of models.

When the ML model is proven correct, it is optimized and used to predict. It is able to determine the best material combinations, defect concentrations, operating temperatures and sensor arrangements that would be the most sensitive and selective. In more sophisticated applications, closed loop systems, ML predictions are used with automated synthesis and characterization systems to discover materials autonomously.

In general, the introduction of ML in the study of gas sensing is a strong platform that could be applied to advance the design of high performance nanostructured sensors. ML can be a major enabler of intelligent, thermoelectric-enabled sensing platforms by providing the opportunity to design intelligent platforms and reduce the burden of experimental work, along with enhancing multi-gas discrimination.



AED: [D2.1]Machine learning optimization of nanostructured gas sensors: The data acquisition and data processing principles (experimental and DFT), feature engineering, model training (ANN/SVM/RF), validation, and prediction of optimal material properties and working conditions.

8. ML-ASSISTED DESIGN OF NANOSTRUCTURED THERMOELECTRIC GAS SENSORS

The three domains of machine learning (ML), nanostructured chalcogenide and thermoelectric sensing convergences have made possible the creation of intelligent gas sensor systems that can be highly selective, low power, and react in real-time. Through ML-based gas sensing systems featured by thermoelectric sensors contrast every standard single-material sensor, hybrid matter architectures and data-directed signal processing that address cross-sensitivity, signal fatigue, and environmental aberration are used to surmount the conventional impairments of such sensors. This combined method is especially useful in the multi-gas detection in complex and dynamic settings.

Hybrid Sensor Arrays with Machine Learning

The hybrid sensor arrays based on a combination of several nanostructured materials, including SnSe 2, WSe 2, Bi 2S 3, and Bi 2Se 3 offer complementary sensing properties because they have different electronic properties, carrier types, and also adsorption energetics. When subjected to a gas mixture, the arrangement of materials in the array produces a distinct pattern of response depending on the interaction of the material and particular gas molecules. The multidimensional response signatures serve as foundations of pattern recognition, which is done by ML.

The collective output of the hybrid arrays can then be processed using ML algorithms such as random forest, support vector machines and neural networks to attain the desired accuracy in the gas classification and the estimation of concentrations. Fusion of features Chemoresistive and thermoelectric signals are merged together using feature fusion techniques, which increase the discriminative ability of the sensing platform. This method decreases the usage of extremely selective solitary materials and allows strong functioning in circumstances with many conflicting gases.

Also the hybrid arrays enhance reliability of sensors by sharing and cross validating signals. When a single sensing element is drifting or deteriorating, the ML models have the ability to counteract it through the use of correlated reactions of other elements. This improves stability in the long-run and lowers the rate of recalibration.

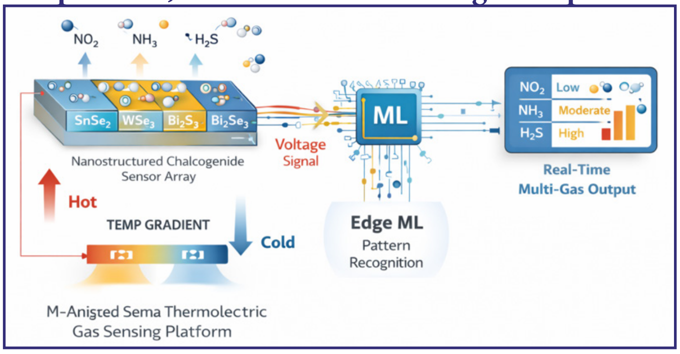
Self-Powered Thermoelectric Sensing with ML Calibration

Certain nanomaterials such as thermoelectric materials can be used to allow self-powered gas sensors, where the temperature gradient causes electrical voltage to be produced. Gas adsorption in such systems changes electrical conductivity and the Seebeck coefficient creating a thermoelectric signal which can be utilized to detect gas without external power on constantly. Nevertheless, temperature variation of the environment and inhomogeneity of materials tend to affect thermoelectric signals.

The compensation of these variations can be effectively achieved with the help of ML-based calibration. ML algorithms can be used to separate the changes in the signal caused by gas and the background thermal effects using temperature-dependent sensing data. This allows the proper detection of gas even in changing ambient conditions.

Moreover, the ML models will be able to determine optimal temperature gradients maximizing the signal-noise ratio and minimizing energy usage. In self-powered systems, this can be used to provide adaptive control of a micro-heater or passive thermal management buildings to achieve the best sensing conditions. This type of smart thermal control has improved sensing performance and power consumption.

Theory [D2.1]Therapeutic Development Therapeutic Development An abstract diagram of an ML-aided thermoelectric gas sensing platform with the nanostructured chalcogenide sensor array, generation of Seebeck voltages by the temperature gradient, edge ML module to identify patterns, and a real time multi-gas output.



Multi-Gas Discrimination Using Pattern Recognition

The ability to discriminate between chemically similar gases with overlapping response signals is one of the major problems in gas sensing. Nanostructured chalcogenides have partial selectivity with respect to adsorption energy and charge transfer processes, but individual sensor values do not produce the reliable, multi-gas detection of a single sensor.

Pattern recognition methods made possible by ML overcome this shortcoming by examining the multidimensional characteristics of response properties, such as response amount, response and recovery rates, thermoelectric voltage change, and signal dynamics. T-distributed stochastic neighbor embedding and principal component analysis are widely adopted as methods of visualization of features and dimensionality reduction, where different clusters can be seen, each one with different gases.

These patterns can then be classified with a lot of accuracy by using supervised learning models. The deep learning structures, especially the convolutional neural networks, can learn to produce more complicated spatial and temporal features of sensor array data. Recurrent neural networks have another benefit in that they are able to capture the time-varying properties of responses and thus identify dynamically the gas.

In this ML-based method, it is possible not only to discriminate gases of like chemical characteristics, like NO 2 and O 3, or NH 3 and amines, but also to discriminate them at low concentrations. It also makes it possible to detect several gases at once which is a requirement in environmental monitoring and other industrial safety applications.

Real-Time Adaptive Sensing

The combination of ML and thermoelectric nanostructured sensors makes it possible to have real-time adaptive sensing systems that can do self-calibration, drift compensation, and optimal response. This is a significant drawback of traditional gas sensors that would result in sensor drift due to age or contamination of materials or environmental modifications. The ML models that are trained on sensing long-term data can detect tendencies of drift and implement the correction transformation to ensure correct gas detection.

Adaptive sensing systems may also adapt parameters of operation on-the-fly depending on the conditions. In the case of temperature gradients, biased voltage or signal processing parameters, the ML algorithms may adjust these parameters to achieve optimal sensitivity and selectivity. The closed-loop process is especially useful in wearable and internet of things-based sensing platforms when conditions in the environment are evolving continuously.

The implementation of Edge ML can enable data processing on the device, which will reduce latency and enable quick gas detection without going to the cloud. This is necessary in safety-critical applications as leak detection and medical diagnostics. Moreover, anomaly detection algorithms can be detected in real time, to detect abnormal gas signatures, which to give early indication of dangerous conditions.

Paramet[D1.1]er	Conventional Approach	ML-Assisted Approach	Outcome
Material selection	Trial-and-error	Data-driven prediction	Faster discovery
Selectivity	Material-specific adsorption	Pattern recognition from arrays	Multi-gas discrimination
Operating temperature	Fixed experimental testing	ML optimization	Lower power consumption
Signal calibration	Manual recalibration	ML drift compensation	Improved stability
Energy efficiency	External power required	Thermoelectric + ML control	Self-powered sensing

9. CHALLENGES AND RESEARCH GAPS

Although machine learning-assisted nanostructured thermoelectric gas sensors have come a long way, there are numerous challenges that impede their large-scale use and practical applications. Availability of high-quality and standardized datasets is one of the major limitations. The majority of the reported studies use small-scale laboratory-level experimental data that are obtained under controlled conditions. The datasets are usually not diverse in the gaseous mixtures, the humidity levels, long term stability, and the real world environmental changes. The fact that there are no large, open-access datasets limits the generalization of models and prevents the creation of workable ML frameworks that can work in dynamic environments.

Another important problem is reproducibility. Differences in synthesis procedures, morphology, defect content, and fabrication of devices cause wide disparities in the sensing ability, even when nominally the same materials have been used. This is where variability causes inconsistent datasets to use in training and validation of ML. Also, sensor performance reporting of sensitivity definitions, response measures and operating conditions are not consistently reported across the studies making cross-comparison and meta-analysis difficult.

The biggest issue is always overfitting, especially when the ML models are being trained on small but high-dimensional data. High accuracy on training data can be obtained by complex models like deep neural networks which cannot generalize to unseen conditions. The small sample of the experiment and absence of systematic validation procedures worsen this problem. These are necessary practices including the application of proper cross-validation methods, feature selection, and model regularization which are not always applied in the modern gas sensing studies.

The unstandardized frameworks of benchmarking are also a hindrance. No standard set of data or testing protocol and performance measure of ML-based gas sensing exists. Consequently, objectivity in comparison of various models and materials becomes quite hard to achieve. A set of benchmark datasets consisting of multi-gas conditions, different humidity conditions and long-term drift data would allow a reasonable comparison and speed up the development of algorithms.

There is an opportunity and a challenge with integration with Internet of Things (IoT) and edge ML platforms. Although thermoelectric nanomaterials can be used to sense passively by operating on a self-powered system, to apply ML models on the low-power edge devices, it is necessary to use an efficient model architecture with lower computational complexity. The existing deep learning systems typically require large amounts of memory and processing capabilities, and these cannot be supported by resource-limited sensor nodes. On-device processing lightweight energy-efficient ML models are open to research.

Another significant impediment is scalability of nanomaterial synthesis. Most high performance nanostructures are made by laboratory scale processes that are not readily scalable to large scale production. To make commercial use of sensors on a large scale, uniform morphology, defect densities, and reproducible thermoelectric properties are required. Moreover, the incorporation of nanomaterials with flexible surfaces and microfabricated thermoelectric surfaces needs sophisticated manufacturing procedures, which are yet to be developed.

To solve these problems, interdisciplinary approaches of the materials science, data science, devices engineering and standardization organizations are required. Creation of large, curated datasets, protocols of synthesis that are reproducible, benchmarking frameworks that are standardized, and edge ML models that are energy efficient will be important in translating research on nanostructured thermoelectric gas sensors aided by ML to real world application.

10. EMERGING TRENDS AND FUTURE DIRECTIONS

The most recent developments show that machine learning coupled with nanostructured thermoelectric gas sensors is heading to autonomous, adaptive, and application-specific platforms of sensing. Use of transfer learning in materials discovery is one of the promising directions. In gas sensing studies, commonly the datasets are scarce in the form of experiments and simple models are easier to train from scratch. Transfer learning allows knowledge acquired on large data sets, e.g., databases of computational materials or other sense systems, to be transferred to new combinations of materials and gases with minimum additional data. High-performance chalcogenide nanostructures can be identified much faster in this way and sensing parameters can be optimized under various operating conditions.

Another trend that is transformative is autonomous laboratories. Closed-loop systems can be used to create, make, and test materials in sensing on a case-by-case basis with the use of ML algorithms, automated synthesis, and testing platforms. These self-directed laboratories have the capacity to sample huge compositional and morphological spaces better than traditional trial-and-error systems, saving time to develop them and enhancing their reproducibility.

Sensor design is no exception as the idea of digital twins is gaining momentum. A digital twin is an online representation of a real device of sensing which incorporates real-time experimental data and predictive models of machine learning. This framework permits the simulation of gas adsorption, charge transport, thermoelectric response, and environmental impacts and optimization of device architecture and operating conditions is possible before physical fabrication. It is also possible to use digital twins to predict maintenance and compensate drift in deployed sensors.

Explainable artificial intelligence (XAI) is necessary to understand the mode of sensing provided by ML models. Though traditional ML models are typically black boxes, XAI methods can be used to understand the role of features, adsorption energetics, and charge transfer pathways which determine sensor response. This interpretability is essential to build faith in ML-aided design and direct reasonable material engineering.

An important area of future development would be the flexile and wearable thermoelectric gas sensor. The low-dimensional chalcogenide nanomaterials in combination with flexible substrate can create lightweight, self-powered sensing devices that can be used in healthcare monitors, occupational safety, and also in environmental exposure monitors. By combining it with edge ML algorithms, it is possible to detect gas in real-time and individually analyze exposure, not relying on external power source or cloud computing.

11. CONCLUSION

The review has presented an extensive discussion about machine learning-assisted optimization of nanostructured chalcogenides, namely SnSe 2, WSe 2, Bi 2S 3, and Bi 2Se 3, used to generate fast and selective multi-gas detection with thermoelectric systems. These materials have unique structural, electronic, and thermoelectric properties, which allow them to be used in next-generation sensing technologies because of the increased gas adsorption, efficient charge transfer, and low-power operation. Nanostructure engineering, defect tuning, and heterostructure creation have been demonstrated to be a large improvement in sensitivity and response dynamics, whereas thermoelectric coupling has been shown to provide self-powered sensing and better signal stability.

Machine learning has come to the rescue as a potent sensor optimization accelerator and has helped to choose material data-driven, extract features, classify gas, predict response, and optimize operating temperature. The cross-sensitivity limitations of the traditional way of working are circumvented with hybrid sensor arrays and multi-gas discrimination within a complex environment is possible with the help of the ML-based pattern recognition. Moreover, ML-assisted calibration and adaptive sensing systems help to improve the long-term stability and minimize the frequent recalibration.

Although this has been done, there are still some constraints such as small datasets, reproducibility, no standard benchmarks, scalability of nanomaterial synthesis and energy-efficient edge ML models. To solve these problems, it will be necessary to design open datasets, evaluations standard protocols, and interdisciplinary teams of materials scientists, data scientists, and device engineers.

Further studies should be done on transfer learning on fast material discovery, closed-loop optimization in autonomous labs, predictive sensor design in digital twins, and explainable AI on understanding the mechanism. Real-time self-powered environmental or health monitoring will also be possible with the further creation of flexible and wearable thermoelectric gas sensors incorporated with edge ML. In general, the integration of nanostructured thermoelectric sensors and machine learning offers the future outlook of intelligent, energy-efficient, and highly selective multi-gas sensing devices.

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