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Artificial Intelligence in Gas Sensing: A Review

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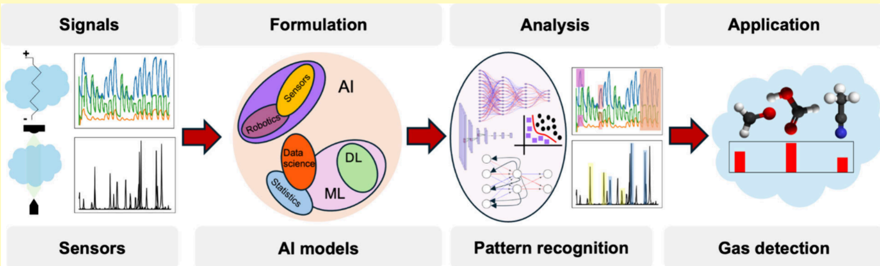

ABSTRACT: The role of artificial intelligence (AI), machine learning (ML), and deep learning (DL) in enhancing and automating gas sensing methods and the implications of these technologies for emergent gas sensor systems is reviewed. Applications of AI-based intelligent gas sensors include environmental monitoring, industrial safety, remote sensing, and medical diagnostics. AI, ML, and DL methods can process and interpret complex sensor data, allowing for improved accuracy, sensitivity, and selectivity, enabling rapid gas detection and quantitative concentration measurements based on sophisticated multiband, multispecies sensor systems. These methods can discern subtle patterns in sensor signals, allowing sensors to readily distinguish between gases with similar sensor signatures, enabling adaptable, cross-sensitive sensor systems for multigas detection under various environmental conditions. Integrating AI in gas sensor technology represents a paradigm shift, enabling sensors to achieve unprecedented performance, selectivity, and adaptability. This review describes gas sensor technologies and AI while highlighting approaches to AI−sensor integration.

KEYWORDS: *Artificial intelligence, machine learning, deep learning, gas sensors, sensing, environmental monitoring, AI−sensor integration, optical, electrochemical, chemiresistive, emerging gas sensors*

Gas sensors are used extensively in various applications, including environmental monitoring, industrial processes, occupational safety, building health, chemical processing, and noninvasive human health monitoring; see Figure 1. For example, gas sensors ensure the safety of workers in mines and chemical factories, detect health conditions based on the concentration of gases in human breath, and monitor greenhouse gas concentrations in the atmosphere.[1−3] Artificial intelligence (AI) refers to the development of computational systems capable of performing tasks that typically require human intelligence, such as recognizing speech,[4] making decisions,[5] analyzing images,[6] and more, by learning from data. AI has revolutionized numerous industries by automating complex tasks and has emerged as a transformative force across numerous fields, enabling computers to uncover hidden insights in large data sets and perform complex tasks that once required human intelligence.[7]

Within AI, machine learning (ML) is a technique that enables these systems to learn from data, recognize patterns, and improve over time without explicit programming. A subset of ML, deep learning (DL) utilizes artificial neural networks (layers of interconnected processing nodes) to automatically extract increasingly complex representations of data.[8] These core concepts work together to power diverse applications, ranging from self-driving cars[9] and virtual assistants[10] to fraud detection[11] and medical diagnosis.[12] For example, AI-powered image recognition systems can diagnose diseases from medical scans with remarkable accuracy,[13] while natural language processing tools are used in customer service and market research to analyze customer sentiment.[14] These applications illustrate how AI not only streamlines workflows but also drives innovation, making it an essential component in solving real-world challenges. Intelligent gas sensing technologies can enhance detection capabilities using AI for signal and pattern recognition.[15] AI-based gas sensor systems can improve performance in existing sensors, allowing improved sensitivity (lower detection limits), selectivity (multigas sensors and fewer

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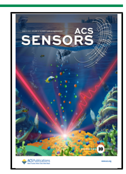

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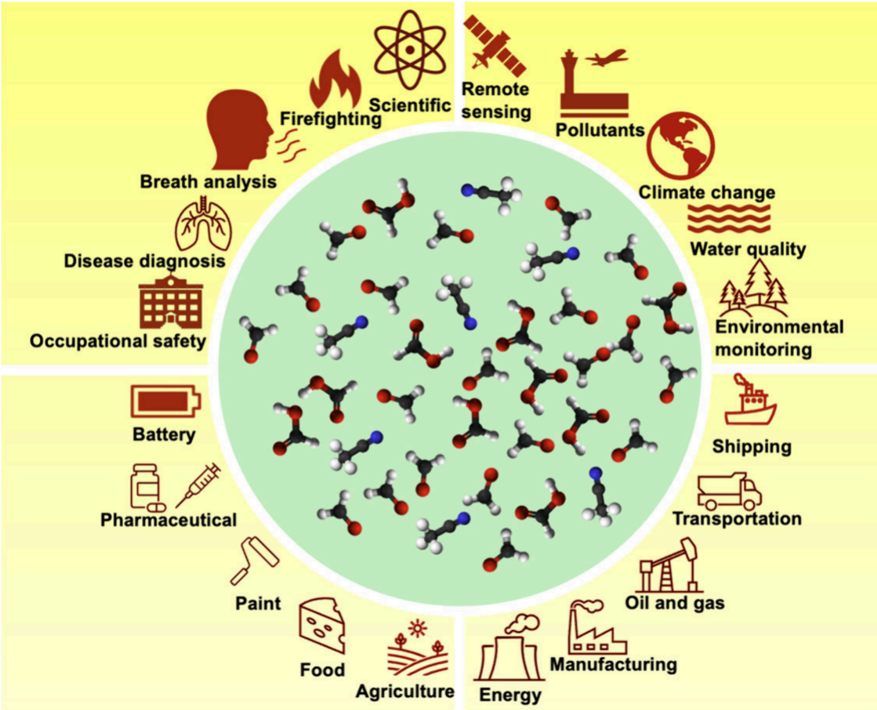

Figure 1. Applications for gas sensors.

false identifications), and time resolution and new gas sensor applications.

Recent reviews underscore the pivotal role of machine learning (ML) in advancing gas sensor technology. For instance, Yaqoob et al. emphasized the urgent need for sophisticated chemiresistive and FET-based gas sensors to tackle pressing environmental and healthcare demands, highlighting how innovative material technologies and ML-driven feature extraction can dramatically enhance adsorption, response, sensitivity, selectivity, and overall sensor intelligence.[16] Ye et al. illustrated how ML-based approaches can significantly improve electronic nose (E-Nose) systems, particularly in odor detection, by enabling both qualitative and quantitative analyses and by mitigating sensor drift to bolster accuracy, reliability, and adaptability across various domains, including robotics, food engineering, environmental monitoring, and medical diagnostics, while also elucidating the role of manual versus learned feature extraction.[17] Similarly, Yang focused on the potential of ML to boost the performance of single gas sensors and sensor arrays, predominantly metal- or semiconductor-oxide-based, for safety and industrial applications such as pollution detection and concentration monitoring, while also discussing ML-based feature extraction and classical algorithms that enhance selectivity, stability, and sensor drift mitigation.[18] Although each of these reviews provides valuable insights into specific facets of ML's role in gas sensor or sensor array applications, the field would benefit from a comprehensive review capturing the rapid progress of AI-driven methods across diverse sensor types, thereby enabling readers to grasp a broader perspective and compare the impact of AI/ML on different gas sensing technologies.

This review is organized to provide a comprehensive overview of gas sensing technologies and their integration with artificial intelligence (AI). We introduce applications of gas sensors in several fields. Following the introduction, the first section introduces various gas sensing methods, including electrochemical, chemiresistive, optical, and emerging sensor types, such as acoustic, liquid crystal, gravimetric, catalytic, and thermal conductivity sensors. Following this, the focus shifts to AI methodologies and their applications in enhancing gas sensing capabilities, with dedicated discussions on AI-based electrochemical sensors, nanoparticle-decorated metal oxide semiconductor (MOS) sensors, electronic noses, optical sensors, and liquid crystal sensors. The integration of AI with emerging gas sensor technologies is explored, emphasizing the challenges of handling large, complex, and multimodal data sets, optimizing feature extraction for high-dimensional data, ensuring physicochemical consistency, and developing trustworthy and interpretable models. The review concludes by addressing the challenges and opportunities in the field.

Emerging Applications for Gas Sensors. Meeting the demand for energy and industrial and consumer goods while minimizing environmental impact is a significant challenge in all regions today. Therefore, one of the largest areas of gas sensor application is monitoring atmospheric air quality and pollutant emissions from industrial sources. The release of pollutants, such as NO_x, NH_3, CH_4, SO_x, CO, volatile organic compounds (VOCs), fluorocarbons, and others, from electricity generation, industrial production, automobile exhaust, and agriculture leads to air pollution, secondary environmental consequences including acid rain, global warming, and ozone layer depletion, and human health issues. Today, gas sensors are addressing air quality and pollutant emissions at local, regional, and global scales, and the continuous monitoring of air quality and local emissions using gas sensors is vital to mitigate environmental and health risks and control air pollution. Many industrial processes, buildings, and remote sensing systems now integrate advanced smart gas sensors to monitor emissions, air quality, worker and occupant safety, and industrial processes. AI-based gas sensor technologies promise improvements in these applications and enable new applications relevant to the environment, human health, and

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industry.[19−24] Intelligent gas sensors utilize a variety of diverse sensor types based on electrochemical,[1] chemiresistive,[25] and optical principles (e.g., absorption spectroscopy), each with unique advantages and challenges from both the hardware and AI integration perspectives.[3,15,26,27]

Human Breath Analysis. Gas sensing for characterizing the composition of human breath has gained traction in recent years as a promising method for medical diagnostics, offering a real-time, noninvasive, and cost-effective way to monitor health. VOCs in human breath can indicate common diseases or health conditions. For example, ammonia, isoprene, and acetone levels in breath samples can help diagnose kidney malfunction, liver fibrosis, and diabetes. Affordable breath analysis holds the potential for widespread clinical application in detecting ailments such as asthma, kidney failure, cancer, diabetes, and heart disease.[28−30] Consequently, there has been significant interest in developing practical VOC sensors for human breath analysis that are cost-effective, easy to fabricate, and capable of operating at room temperature with high sensitivity and selectivity.[31] VOCs are also emitted from natural sources and human activities, impacting indoor and outdoor air quality, and serve as markers in various applications, such as disease detection, fruit ripening, and explosive detection. Hence, VOC detection is of broad interest in gas sensing.

Battery Health Monitoring. With the increased reliance on batteries for energy storage in applications such as electric vehicles, renewable energy systems, and portable electronics, ensuring battery health and safety has become an urgent priority.[32] Failures in batteries, particularly thermal runaway (a condition where internal heat generation leads to uncontrolled reactions), can result in catastrophic outcomes such as fires or explosions.[33] Current battery monitoring methods often fall short in detecting early warning signs of such failures, leading to increased safety risks and reduced battery performance, and require innovative, real-time monitoring solutions capable of predicting and preventing faults before they escalate.[34] During battery failures, vapor electrolytes and products of the combustion of the electrolyte are often produced and detectable in the gas phase which can be detected using electrochemical, chemiresistive, optical, and other sensors.[35] A potential solution to this problem lies in intelligent gas sensing, enhanced by AI. AI can learn from complex and dynamic data sets produced by gas sensors and identify subtle patterns and anomalies, offering early detection of potential failures and can enhance safety while also allowing for more efficient maintenance, reducing downtime and extending battery life.[35] The released gases serve as chemical fingerprints of internal battery issues, providing valuable diagnostic information. Recent advancements in AI-assisted smart sensor strategies have demonstrated their potential to address these challenges.[36] By integrating sensors with AI, researchers are developing systems that can proactively monitor battery health, detect faults early, and provide actionable insights for safety and reliability.[37] This approach represents a significant step forward in creating robust, efficient, and safe energy storage systems, which are essential to supporting the increasing demand for sustainable and reliable energy solutions.[38]

Food Quality. ML algorithms have been used with E-nose systems to monitor food and beverage quality, including the freshness and quality of meat, fish, dairy products, chocolate and cocoa, alcoholic beverages, tea and coffee, and oils and vinegar, demonstrating the potential of AI-based intelligent electronic nose systems to sensitively and selectively monitor trace gases at low cost to provide nondestructive quality control methods across the food sector.[39,40]

Water Quality. Gas sensors can help ensure the safety and compliance of water treatment facilities by monitoring odors and detecting toxic and flammable gases, such as hydrogen sulfide, methane, and carbon monoxide, common byproducts of organic decay in water. In this environment, real-time, sensitive, and selective gas sensing is required for continuous monitoring. To date, improvements in hardware have allowed the development of sensors that meet the requirements of water quality applications.[39,41,42] The transition to digital tools and technologies, including AI-based gas sensors, has the potential to provide a step improvement in water quality management systems. The focus on AI-based solutions in water quality reflects a broader trend toward leveraging new AI and data technologies to address environmental management issues.[41,42]

Robotics and Automation. Mobile robots that mimic human capabilities require sensory systems such as vision, hearing, and smell. Gas sensor arrays, or electronic noses, can provide a robotic olfactory system to identify different gases. By combining electronic noses with AI, robots can analyze gas patterns, create a “smell print”, and enable environmental monitoring, food safety, and health diagnostics applications.[12,16,43] Recent advances focus on improving electronic nose fabrication, flexibility and weight, sensitivity, and AI integration and their integration into robots, including drones and wearables. From a robotics perspective, integrating electronic noses into robots significantly enhances their autonomy and utility in complex environments, opening possibilities for new applications. Furthermore, applying AI to process and interpret the complex data produced by electronic noses increases the intelligence and autonomy of these robotic agents. The convergence of advanced materials, sensor technologies, and AI represents a significant step toward creating more responsive and adaptive robotic systems.[12,43]

Gas Sensor Performance Metrics. Various critical metrics determine gas sensor performance, each defining some aspect of a sensor’s effectiveness for detecting gases under different conditions. These performance metrics include sensitivity, selectivity, stability, response time, energy consumption, and others, all of which are essential for achieving reliable and practical real-time gas detection in fields such as environmental monitoring, industrial safety, and medical diagnostics.[44] Sensor materials and design advances continually enhance these attributes, making modern sensors more efficient and reliable.

Sensitivity defines the lowest concentration of a gas that a sensor can reliably detect, represented by the change in the output signal relative to the baseline per unit concentration of the target gas. A steeper response curve indicates higher sensitivity, crucial for detecting trace gases.[25] Selectivity measures the ability of a sensor to distinguish a specific gas in a mixture, reducing cross-sensitivity and false readings. Techniques such as combining multiple sensing materials enhance selectivity by lowering the activation energy for specific gas interactions.[45,46]

Response time is required for a sensor to reach a specified percentage of its final output after exposure to a target gas, with fast response and recovery times being crucial for real-time monitoring. Stability refers to the sensor’s ability to maintain consistent performance over time, influenced by grain size,

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pore structure, and chemical composition.[22] Energy consumption is vital for portable or battery-powered devices where low-power sensors are preferred.

Other important metrics include repeatability, the sensor's ability to produce consistent results under identical conditions, and reversibility, which describes its ability to return to its baseline state after exposure. Hysteresis refers to the variation in output when the gas concentration changes, and minimizing this ensures accurate readings. Dynamic range and resolution relate to the sensor's ability to detect a wide range of gas concentrations and small concentration changes, respectively.[47]

Operating temperature and fabrication costs are also critical in sensor design. Sensors that operate at room temperature have lower energy consumption, but some, like metal oxide sensors, require higher temperatures for optimal performance.[25] Miniaturization and detection limits are increasingly significant, particularly in wearable technology and portable devices, driven by innovations in nanomaterials and surface treatments.[22]

Gas sensor performance hinges on a combination of performance metrics, and advancements in sensor technologies continue to address and improve these metrics, making modern gas sensors more reliable, efficient, and suitable for diverse applications, from industrial safety to healthcare.

Gas Sensor Market. The gas sensor market has grown significantly, fueled chiefly by increasing air pollution, monitoring air quality,[48] and broader applications for gas sensors in healthcare.[16] In the next decade, Dhall et al. project the gas sensor market will grow at a compound annual growth rate of 7.5%;[20] see Figure 2. Asia Pacific is the largest market at 35%, followed by Europe at 27%, and North America at 23%.[49] Gas sensor manufacturers with large market share include Alpha MOS, ABB Group, Delphi Automotive PLC, The Bosch Group, Emerson Electric Co., Denso Corporation, Halma plc., Honeywell International Inc., Siemens AG, F. Hoffmann-La Roche Ltd., Yokogawa Electric Corporation, Dynament, Figaro Engineering Inc., AlphaSense Inc., City Technology Ltd., Membrapor, Nemoto & Co. Ltd., GfG Gas Detection UK, FLIR Systems, and Robert Bosch LLC.[49−51]

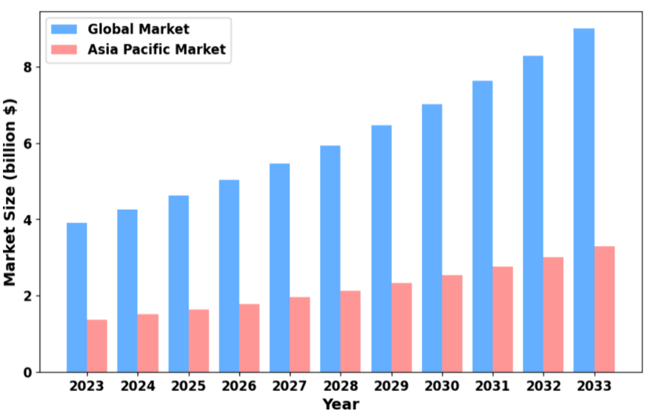

Figure 2. Gas sensor market projections.[49]

Opportunities for AI in Gas Sensing. The development of gas sensing technologies has concentrated on three key areas: sensing methods, sensor materials and design, and sensor fabrication.[22] Traditional gas sensing approaches and technologies can face challenges owing to the fundamental limitations of their methods, materials, design, and fabrication. Limitations may include lack of selectivity or reproducibility, limited sensitivity, drift, performance degradation over time, restricted performance at high or low temperatures, and energy consumption.[21] AI-based approaches and improvements in materials and sensor technologies can improve gas sensing methods to address these and other challenges.

Applying AI, ML, and DL to gas sensor technologies can significantly improve their sensitivity and selectivity. By processing and analyzing the data collected from gas sensors, AI algorithms can detect small signals, separating them from noise or competing gas signatures that traditional methods and algorithms cannot detect, thereby increasing the sensitivity and selectivity. Gas sensor systems often generate large volumes of data. Because AI, ML, and DL can efficiently analyze high-dimensional data sets, they can simultaneously identify patterns and trends in data streams, enabling gas sensor networks or arrays that provide significantly more information than stand-alone sensors or combinations of stand-alone sensors.[52] With the help of AI and ML, gas sensor systems can process data in real-time, often in a compressed or encoded form, providing immediate real-time alerts and enabling quick decision-making, which is crucial in hazardous situations.[53,54] AI and ML models can also help sensors adapt to changes in environmental conditions, including temperature, pressure, and humidity, and can also help to deal with sensor signal degradation (e.g., drift). Hence, AI-based systems can offer more information (e.g., detection of many species), automation, intelligence, and reliability in gas sensing for environmental monitoring, industrial safety, and other applications.[15]

AI and ML models are well suited for processing dynamic sensor signals and detecting unique patterns associated with gases, and therefore, ML has emerged as a tool for improving gas sensors. Additionally, by implementing ML approaches to signal processing, sensors can be realized using less expensive hardware. For example, sensor systems have moved toward compact arrays of nano/microsensors integrated on single flexible substrates rather than combinations of independent, stand-alone sensors.[16] ML techniques enable the integration of data mining, pattern recognition, and classification with gas sensors, enabling the fusion of sensors and information technologies in practical applications such as environmental monitoring.[55]

The application of AI, ML, and DL in gas sensor development addresses the limitations of traditional gas sensors and methods. These technologies can significantly improve the gas sensor sensitivity, selectivity, reliability, and time resolution. Hence, AI-based gas sensors can offer a paradigm shift, enabling improved performance and new applications. This review describes state-of-the-art gas sensor technologies as well as recent examples and future approaches to integrating AI into gas sensor systems.

GAS SENSING METHODS AND TECHNOLOGIES

Typically, the most critical performance factors for gas sensors are sensitivity, selectivity, response time, and stability. Advances in materials science, nanotechnology, optics, and micro- and nanofabrication techniques have improved these parameters for various gas sensor systems. Gas sensors can be broadly categorized into several types, each with unique working principles and technologies. Here, we will focus on electrochemical, chemiresistive metal oxide semiconductor,

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and optical gas sensors, which are widely developed commercially. We will also describe several categories of sensors that are still under technological development, including acoustic sensors, sensor films composed of functional materials, liquid crystal, gravimetric, catalytic, thermal conductivity, and conducting polymer sensors. Figure 3 illustrates several gas sensor types and their operating principles.

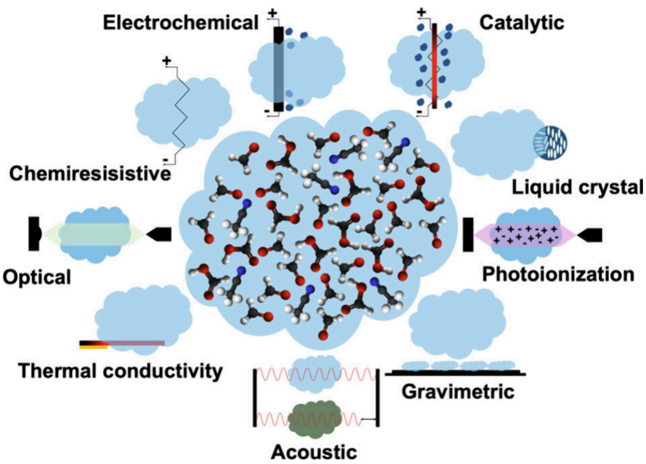

Figure 3. Common types of gas sensors.

Electrochemical Gas Sensors. The oxidation or reduction of target gases at an electrode can generate a current proportional to the gas concentration. This electrochemical principle can be harnessed to produce high-sensitivity and specificity gas sensors, as first demonstrated by Taguchi.[56] Electrochemical gas sensors are favored for their low power consumption, ideal for portable devices, and are commonly used to detect small molecule gases, including CO, H_2, and SO_2.[57] An electrochemical sensor consists of a cell with two or three electrodes: a reference, a working, and sometimes a counter electrode separated by an ionic conductor. Gas detection occurs through oxidation or reduction reactions on the working electrode, creating a measurable electric current. This reaction, involving the transfer of electrons through external wiring to the counter electrode, allows the sensor to quantify gas concentrations effectively, functioning similarly to a battery. Electrochemical gas sensors are often inexpensive and portable but typically have a shorter lifespan than other gas sensors.[20]

Chemiresistive Gas Sensors. Chemiresistive gas sensors operate by detecting changes in the electrical resistance of a sensing material upon exposure to a target gas. This fundamental principle has made these sensors a cornerstone of gas detection technology since their commercial introduction in the 1960s. Metal oxides have been the predominant materials used as the sensing layer in chemiresistive gas sensors. These metal oxide semiconductor (MOS) gas sensors are highly regarded for their sensitivity (capable of detecting gases at parts per million to parts per billion levels), rapid response and recovery times, ease of fabrication, stability, simplicity, and cost-effectiveness.[23] Due to these important performance features, MOS gas sensors have been widely developed commercially and applied in many applications. Despite their advantages, MOS sensors typically require high operating temperatures, leading to high energy consumption.[15] Moreover, their selectivity in mixed gas environments can be limited, prompting ongoing research into improving response selectivity through structural and surface modifications.[45]

The chemiresistive effect, characterized by changes in electrical resistance in the presence of gases, is directly correlated with variations in the gas concentration. The effect was first explored with materials like germanium and zinc oxide[58,59] and has since expanded to many metal oxides.[44,60,61] Traditionally, chemiresistive sensors consist of an insulating substrate, interdigitated electrodes, and a heater to maintain operational temperatures, typically ranging from 100 to 450 °C. However, these high temperatures require high power inputs and present challenges in long-term stability.[23]

The functionality of chemiresistive sensors relies on the resistance modulation of a material when it is exposed to target gases. This chemiresistive effect leads to the formation of electron depletion or accumulation layers on the sensor's functional material surface. To engineer a chemiresistive gas sensor for quantitative gas concentration measurements, engineering the functional sensing material, where the chemiresistive effect takes place, is critical for optimal sensor performance.[62] Nanostructures often enhance the sensing process, allowing a high surface-to-volume ratio for contact with target gases and improved performance. Recent research has focused on improving the sensing layers using conventional metal oxides, emerging nanocomposites, and graphene-like two-dimensional materials.[2]

MOS sensors, such as those made from tin oxide (SnO_2), titanium oxide (TiO_2), indium oxide (In_2O_3), tungsten oxide (WO_3), and zinc oxide (ZnO), operate based on reactions between chemisorbed oxygen species and analyte gases, altering the sensor's electrical resistance. While sensitive, tin oxide-based sensors often suffer from slower response times, lower selectivity, and higher operating temperatures. Surface decoration with metal nanoparticles has been explored to improve the MOS gas sensor performance. The deposition of nanoparticles such as Au, Pd, or Pt enhances sensitivity by increasing adsorption capacity and forming Schottky barriers, enabling the detection of gases at parts per billion levels.[63−66]

MOS sensors are typically porous polycrystalline materials, where the surface of metal oxide grains acts as the receptor and the grain boundaries serve as transducers. The gas diffuses into the sensor through a porous membrane, causing a chemical reaction that changes the film's physical properties and alters electrical resistance. The metal oxide layer is often doped with small amounts of foreign substances known as sensitizers, such as noble metals or their oxides.[1] The ongoing development of these gas sensors focuses on using materials with high stability and low oxidation to extend sensor lifespan and enhance performance, making them valuable for a wide range of applications from health to environmental monitoring.[20] Additionally, additives to chemiresistive materials, such as metals and conductive polymers, have proven effective in further enhancing these sensors by increasing the charge carrier concentration and reducing the activation energy needed for sensing.[67]

Nanomaterials are often used in the development of MOS gas sensors. The effectiveness of a nanoscale gas sensor largely depends on its nanostructure and morphology, which are typically optimized using surfactants. Four primary strategies to enhance the application and performance of MOS gas sensors include controlling the nanostructure, doping with nanomaterials, decorating with noble metal nanoparticles, and forming heterojunctions.[61]

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The dimensionality of the nanomaterials used primarily classifies nanomaterial-based gas sensors. Zero-dimensional (0-D) nanomaterials include carbon dots, nanoclusters, and metal nanoparticles. One-dimensional (1-D) nanomaterials, such as nanowires and nanotubes, are also widely used. For example, silicon nanowires (SiNWs) can be chemically functionalized to selectively detect specific gases and operate efficiently at room temperature, offering advantages over metal oxide nanowires, which typically require higher operating temperatures or UV light.[68] Two-dimensional (2-D) nanomaterials, such as graphene derivatives, MXene derivatives, metal−organic frameworks (MOFs), and covalent organic frameworks (COFs), have also been extensively studied.[44]

Nanostructures like nanorods, nanobelts, and nanofibers have been demonstrated in detecting hazardous gases like NO_2, NH_2, and H_2S.[25] Emphasis on computational and experimental methods to determine optimal gas molecule adsorption sites, including bandgap tuning through nanostructures and metal/metal oxide catalytic reactions, is necessary. Such approaches will enhance the integration of ML techniques for sensor data analysis and further improvement.[16]

Each nanomaterial type brings specific advantages to gas sensors. For instance, carbon nanotubes (CNTs) and graphene offer a high surface-to-volume ratio, significantly enhancing gas molecule adsorption and sensitivity. Metal oxides are favored in solid-state gas detectors for their stability and cost-effectiveness. Furthermore, 1-D metal oxide nanostructures have been demonstrated for their ability to improve sensor performance through enhanced electrical contacts and efficient gas molecule interactions.

CNTs play a pivotal role in the development of chemiresistive sensors, leveraging their exceptional electronic, mechanical, and chemical properties to create highly sensitive and selective devices.[69] They are highly sensitive to their electrical environment, making them promising candidates for gas sensors.[70] Their electrical properties change significantly upon exposure to certain gases, although their sensitivity is limited to molecules with large binding energies and charge transfer interactions with the nanotubes.[1] CNT-based sensors have been reported for detecting various gases, including NO_2, H_2S, H_2O_2, H_2, CO_2, CH_4, NH_3, Cl_2, ethanol, and trinitrotoluene.[46] CNT gas sensors have been developed based on single-walled (SWCNTs) and multiwalled (MWCNTs) types, and they have been applied in both pure and composite forms for gas detection.[71] Luo et al. have analyzed and assessed the potential and challenges of CNT-based sensors for various applications, including environmental monitoring, industrial safety, and healthcare. Their work highlights the need for enhanced sensitivity, fast response, and low power consumption to offer high selectivity and robust, reliable CNT-based sensors.[72]

Advanced nanostructures, including CNTs, nanowires, and hollow spheres, have demonstrated promise in detecting various gases at various concentrations. Functionalizing CNTs with MOS materials, for instance, enhances sensitivity, particularly for detecting NO*x* gases at low temperatures. Recent advancements highlight their potential in gas sensing applications, demonstrating attributes like fast response, low power consumption, and adaptability to miniaturized and integrated designs.[72] CNTs can operate effectively at room temperature but are sensitive to humidity.[15] Incorporating ML techniques enhances the selectivity and stability of CNT-based sensors, broadening their utility in innovative applications include breath analysis for medical diagnostics, where CNTs are integral to developing electronic noses, enabling the detection of disease biomarkers with statistical methods and rigorous experimental validation.[73] Additionally, emerging techniques for CNT-based gas sensors have shown success in detecting specific gases like ammonia and ethylene, achieving high sensitivity and selectivity under ambient conditions.[74]

Recent research has also focused on the exploration of 2-D nanomaterials. Improvements aim to increase the selectivity and sensitivity of the sensors while reducing their operational power requirements. 2-D nanomaterials, such as graphene and its derivatives, have been rigorously explored for chemiresistive gas sensing due to their exceptional surface-to-volume ratios, lower operating temperature, and intrinsic properties conducive to high-performance sensor applications. This research has investigated various gas sensing mechanisms, such as adsorption and charge transfer, and has explored their incorporation into different types of devices, including field-effect transistors (FETs) which enhance sensitivity by modulating graphene's conductivity through a gate voltage, making them highly sensitive for applications such as gas leak detection.[15,75−78]

Graphene oxide, due to its versatile properties and suitability for being doped with nanoparticles has been shown to facilitate the detection of a diverse array of gases including nitrogen dioxide, hydrogen, ammonia, hydrogen sulfide, and various organic vapors.[79−83] By integration of diverse functionalization strategies and artificial intelligence, rapid detection of VOCs with functionalized sensor arrays[77] and precise vapor discrimination in humid conditions using DNA-functionalized graphene have opened up avenues for new sensing applications.[78] Chemiresistive sensors based on MoS_2 nanoflakes with defects and exposed-edge sites aided with several machine learning models for highly accurate, selective, and sensitive trace gas detection of triethylamine among VOCs have been reported recently.[84] The use of transition metal-doped tungsten diselenide (TM-WSe_2), a 2D material, for detecting greenhouse gases (CO_2, CH_4, N_2O, SF_6) has efficiently screened 28 TM-WSe_2 configurations in a recent study exhibiting the potential of future sensor development based on transition metal dichalcogenides.[85]

Researchers have also explored doping or decorating the nanostructures to enhance gas sensing properties further, offering more refined control over the sensor characteristics. Among these methods, noble metals are favored for their superior performance, despite their higher cost. New nanostructures, including nanowires, nanotubes, core−shell structures, nanoneedles, nanosheets, and nanofibers, have become prominent in developing MOS devices due to their large surface-to-volume ratios. Specifically, MOS nanowires have been extensively researched for their potential to detect toxic gases, showing superior sensing properties compared to their bulk or thin film counterparts.[86] Heterojunctions are also widely used because they combine different materials to leverage performance benefits, and they are relatively simple and cost-effective to prepare.[87] However, there is still substantial room for improvement across all of these methods. For practical application, material stability in the target gas environment is crucial, as are properties like large surface-to-volume ratios and ease of preparation.[61]

The advent of novel nanomaterials has increasingly driven the development of gas sensor technologies. These materials offer unique electrical, optical, and mechanical properties,

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making them suitable for creating sensitive and low-power sensors. However, challenges remain in transitioning from laboratory research to practical, real-world applications, particularly in integrating these sensors with microelectronics and AI for enhanced performance.[88] In terms of technological integration, the transition toward wireless gas sensing systems is also critical, leveraging the properties of these nanomaterials to achieve compact, efficient sensors with broader application scopes, including remote real-time monitoring capabilities in diverse environments. Such wireless remote gas sensors, integrating advanced transducers that are engineered to operate under varying conditions without losing efficacy, may be appropriate for the integration of AI methods to improve performance and provide autonomy.[89−93]

Optical Gas Sensors. Optical gas sensors have found implementation in modern smart sensing platforms and are widely used in areas such as process monitoring, quality prediction, pollution control, defense, and security. Optical gas sensors employ techniques such as light absorption, luminescence, fluorescence, reflectance, or scattering to detect gases, offering high sensitivity and reduced susceptibility to electrical noise, making them ideal for harsh environments where noninvasive gas detection may be beneficial or required over the contact methods inherent to electrochemical and chemiresistive sensors. Most commercial optical gas sensors rely on optical absorption at specific wavelengths where rotational, vibrational, or electronic transitions exist and include a radiation-emitting element (e.g., laser) and a photon-detecting element (e.g., diode photodetector). Small molecules such as CO, CO_2, H_2O, NO, NO_2, NH_3, and CH_4 have been widely detected using optical gas sensors,[94−96] more specifically via absorption spectroscopy, and larger VOCs such as alcohols, benzene, toluene, xylene, and others can be detected via optical gas sensors with high sensitivity across a wide range of temperatures and even in challenging environments.[97]

Optical spectroscopy is crucial in detecting VOCs and is vital for monitoring air quality and diagnosing diseases. Recent advances in nondispersive infrared (NDIR) spectroscopy, multipass cell spectroscopy, cavity-enhanced absorption spectroscopy, photoacoustic spectroscopy, and Fourier transform infrared spectroscopy have significantly improved the sensitivity and selectivity required for effective VOC detection. Advances have focused on improving detection limits by system parameters, such as optical source power and wavelength, and overcoming design challenges in integrating these technologies into compact, efficient sensors. The importance of low-cost, high-resolution air quality sensors has become especially apparent due to increasing concerns over public exposure to air pollution and also the increased importance of indoor air quality and their links to respiratory health.[98−100]

Infrared (IR) absorption gas sensors detect gases based on the spectral absorption of incident radiation. These systems utilize an IR radiation source and detector to detect a target gas along a line-of-sight path. They can use the Beer−Lambert law to determine the path-averaged concentration of the target gas. IR gas sensors may also utilize optical fibers, which can be dispersive (using gratings or prisms) or nondispersive (using discrete optical band-pass filters, commonly used in gas sensors) to direct radiation. They may also feature a gas cell that allows the light path to interact with the target gas and can provide multiple radiation passes to increase the path length. IR gas sensors effectively detect small molecule gases and some large molecules, including VOCs, as long as the target molecule contains a dipole moment in the rovibrational energy structure, providing spectroscopic transitions at the frequency of the incident radiation with sufficient strength.

IR gas sensors have been developed around a variety of optical structures to improve performance, including multibeam and multiwavelength configurations for noise reduction,[1] integrated cavity output spectroscopy cells that allow multiple passes that increase the optical path length to many times the physical cell path,[101] and cavity ring-down spectroscopy which implements pulses of incident radiation that are trapped in a highly refined optical cavity to increase the effective optical path length.[102]

Terahertz (THz) frequency (0.1−10 THz) absorption gas sensors have shown promise in addressing the challenge posed by water vapor interference, which complicates gas detection in the IR, where water vapor has a significant and strong absorption and can interfere with target features for other gases. THz sensors are increasingly used in noninvasive, contactless gas sensing, taking advantage of their ability to penetrate opaque materials. THz time-domain spectroscopy, one form of THz absorption, delivers short, broad-spectrum THz pulses that pass through various materials, providing amplitude and phase information on the reflected or transmitted THz waves. This information can be used to identify gases at low concentrations and to identify and measure properties for solids and liquids. The ability of THz waves to differentiate between materials, particularly polar gases, based on their spectral fingerprints enhances their utility in complex material systems, gas mixtures, and composites found in modern industrial applications.[19,103]

Over the past decade, ML and DL have significantly advanced optical gas sensor applications, increasing sensitivity and selectivity and providing automation. Despite their advantages, optical gas sensors face significant challenges, including their complexity in application relative to chemiresistive gas sensors, the generation of large data sets, which results in slow data processing speeds, and high costs. However, optical gas sensors provide noninvasive sensing, which other technologies cannot provide. Integrating AI, ML, or DL methods with optical sensors offers solutions to signal processing limitations. Recent studies highlight the potential of DL models, particularly deep neural networks (DNNs), to improve the functionality of these sensors. DNNs have shown promise in dynamically extracting features from raw data with high accuracy, often surpassing human capabilities. DL models enhance the performance and reliability of optical sensor systems by processing vast data sets, preprocessing noisy data, automating feature extraction, and providing reliable predictions.[104]

Emerging Gas Sensor Types. *Acoustic Gas Sensors.* Acoustic gas sensors measure changes in the acoustic properties of a gas, which are influenced by its concentration. These sensors are categorized into several types, each utilizing distinct mechanisms for gas detection. Surface acoustic wave (SAW) sensors are highly sensitive and detect changes in mass when gases are adsorbed onto their surfaces, thereby altering the properties of acoustic waves traveling along the surface. The interaction with gas molecules affects the velocity or amplitude of these waves, allowing for the precise measurement of gas concentration. SAW sensors incorporate interdigital transducers that are crucial for generating and

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receiving acoustic waves. The sensitivity of SAW sensors enables the detection of various gases at low concentrations, making them valuable in applications such as food quality assessment, where they analyze produce types, taste profiles, and shelf life. Advances in integrated circuit technology have made these sensors more compact, multifunctional, and portable, enhancing their applicability across diverse fields. Additionally, ongoing research is focused on improving the materials and sensitivity of SAW sensors, reducing production costs, and integrating biomolecules for enhanced gas detection capabilities.[40]

Quartz Crystal Microbalance (QCM) gas sensors measure the change in the frequency of a quartz crystal resonator when gas molecules adsorb onto its surface. This adsorption increases the mass of the crystal, leading to a decrease in its resonating frequency, which is proportional to the mass of the absorbed gas. This characteristic makes QCM sensors particularly effective for detecting VOCs and other gases at low concentrations with high sensitivity. Moreover, QCM/SAW sensors are recognized for their precise humidity detection capabilities.[15] Bulk acoustic wave (BAW) sensors operate similarly to SAW sensors but differ because the acoustic waves travel through the bulk of the material rather than just along its surface. The interaction with gas molecules causes changes in the wave properties, enabling the detection of the presence and concentration of the gas. BAW sensors are often more robust than SAW sensors under certain conditions and find use in similar applications.[105]

Acoustic resonance gas sensors detect changes in the acoustic resonance characteristics of a cavity or chamber, which the presence of different gases can influence. The resonance frequency or damping of acoustic waves within the chamber changes depending on the type and concentration of the gas, facilitating gas detection and quantification. Acoustic gas sensors, including SAW, QCM, BAW, and resonance sensors, have wide-ranging applications such as detecting pollutants or hazardous gases, monitoring toxic or explosive gases, analyzing breath for biomarkers in medical diagnostics, and monitoring exhaust gases or cabin air quality in the automotive and aerospace industries.[105]

Liquid Crystal. Liquid crystal (LC) materials may present advantages over traditional MOSs for gas sensors including fast and reversible optical responses, low energy consumption, and operation at room temperature. When a gas of interest interacts with the LC, it can cause a change in the orientation or alignment of the LC molecules. This interaction can be due to physical absorption, chemical reaction, or other mechanisms depending on the type of LC and gas.[106] These properties have made LC materials attractive for developing rapid, miniaturized, and low-cost gas sensor devices. Research has particularly focused on hybrid gel films containing LC droplets, which exhibit characteristic optical texture variations due to the orientational transitions of LC molecules when exposed to different VOCs.[107] LC-based sensors are especially valuable in areas such as occupational health, homeland security, and medicine, where wearable and lightweight sensors are paramount. While traditional metal oxide and electrochemical sensors are sensitive, they often fail to meet regulatory compliance standards due to issues of stability and reliability in certain applications. In contrast, LCs, which possess properties of both crystalline solids and isotropic liquids, offer a promising alternative for wearable sensors, including badges designed to monitor toxic gas exposure.[108]

Gravimetric Gas Sensors. Gravimetric gas sensors detect mass changes, which occur when gas molecules adsorb onto the sensor's surface. This mass change directly influences the sensor's output, making these sensors effective for gas concentration measurements. The most common type of gravimetric gas sensor is the quartz crystal microbalance (QCM). QCM sensors operate on the principle of a quartz crystal vibrating at a specific frequency. When gas molecules adsorb onto the crystal surface, they increase the mass of the crystal, resulting in a measurable shift in its vibration frequency. This frequency shift is directly proportional to the mass of the adsorbed gas molecules, allowing for precise quantification of the gas concentration.[109] The high sensitivity and accuracy of QCM sensors make them particularly suitable for detecting low concentrations of gases, including VOCs and other trace gases in various environments.[110]

In addition to their sensitivity, QCM sensors offer several advantages, such as their ability to operate under ambient conditions and relatively simple and robust design. These characteristics make them ideal for applications in environmental monitoring, industrial safety, and medical diagnostics, where detecting and quantifying minute amounts of gases is crucial.[109] Furthermore, ongoing research is focused on enhancing the performance of QCM sensors by improving their surface coatings and integrating them with advanced signal processing techniques, thereby expanding their application range and improving their reliability in complex sensing environments.[110] As a result, QCM sensors continue to play a vital role in developing next-generation gravimetric gas sensing technologies.

Catalytic Gas Sensors. Catalytic gas sensors can detect flammable gases, allowing their application in industrial safety, environmental monitoring, and residential gas detection.[15] When exposed to a target gas, these sensors catalyze a chemical reaction on their surfaces, generating heat. This heat increases the temperature of the sensor's surface material, changing its electrical resistance. The sensor then measures this resistance change to determine the concentration of the gas present.

Catalytic gas sensors are reliable and can detect a wide range of flammable gases including methane, propane, and hydrogen. Their wide applicability in hazardous environments underscores their importance in preventing accidents and ensuring safety. Despite these advantages, catalytic sensors do have limitations. They require the presence of oxygen to function effectively, which can limit their use in oxygen-deficient environments. Additionally, these sensors are susceptible to sensor poisoning by certain chemicals, such as silicones or sulfur compounds, which can degrade the sensor's performance over time. Regular calibration is also necessary to maintain accuracy, especially in environments where sensor drift may occur due to prolonged exposure to target gases or contaminants.

Photoionization Detectors. Photoionization detectors (PIDs) can detect VOCs and other gases by utilizing ultraviolet (UV) light to ionize gas molecules. When the gas molecules are exposed to UV light within the sensor, they absorb energy and become ionized, releasing electrons. The sensor then measures the flow of these ions, which is proportional to the concentration of the gas present. PIDs can be sensitive and capable of detecting low levels of VOCs, often in the parts per billion (ppb) range, making them valuable in applications where even trace amounts of hazardous compounds must be detected. These applications

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include environmental monitoring, industrial hygiene, leak detection, and hazardous materials response.

One of the significant advantages of PIDs is their ability to detect a broad range of organic compounds, including benzene, toluene, and xylene, as well as some inorganic gases, such as ammonia and hydrogen sulfide. Additionally, PIDs offer real-time monitoring and rapid response times, which are critical in preventing exposure to harmful levels of VOCs and ensuring workplace safety.[111] However, PIDs are generally nonspecific, meaning they cannot distinguish between different types of VOCs and their response can be affected by humidity and other environmental factors. Additionally, PIDs require regular maintenance, such as cleaning the UV lamp and calibration, to ensure a consistent performance. Advances in PID technology continue to focus on improving their selectivity, sensitivity, and durability in challenging environments, thereby expanding their applicability and reliability.[112]

Thermal Conductivity Gas Sensors. Thermal conductivity gas sensors operate by detecting changes in the thermal conductivity of a gas mixture. These sensors typically consist of a heating element and temperature-sensitive components, such as thermistors and resistance temperature detectors. When a gas flows through the sensor, it alters the rate at which heat is conducted away from the heating element. This change in heat dissipation causes a corresponding change in the temperature of the sensor's components. The sensor measures this temperature variation and correlates it with the target gas concentration.

Thermal conductivity sensors effectively detect gases whose thermal conductivities differ significantly from the background gas such as hydrogen, helium, and carbon dioxide. Due to their ability to measure absolute gas concentration, these sensors are used in applications such as gas leak detection, process control in industrial settings, and respiratory monitoring in medical devices.[113] One of the key advantages of thermal conductivity sensors is their simplicity and robustness, allowing them to operate under a wide range of environmental conditions with minimal maintenance. However, thermal conductivity gas sensors are generally nonselective, meaning they cannot distinguish between gases with similar thermal conductivities. Their accuracy is influenced by environmental factors, such as changes in ambient temperature, which necessitate frequent calibration. Research aims to address these challenges by developing new materials and sensor designs that enhance selectivity and stability.[2]

■ ARTIFICIAL INTELLIGENCE METHODS

Gas sensors generate signals that require processing and interpretation to detect and quantify the target gases. AI methods are particularly effective for these tasks, offering robust solutions for various signal processing and interpretation functions. Additionally, AI enables adaptive and autonomous operation and allows for real-time sensor performance optimization. This includes adjustments to sensor operations in response to environmental conditions, signal characteristics, or other parameters.

Before the emergence of modern deep learning based AI, gas sensing relied on chemometric methods including PCA, MCA, ICA, SMCR, and PLS, along with empirical models using calibration curves or regression to analyze sensor responses.[114−120] Practitioners started distinguishing these traditional methods from ML in the late 1980s since these methods were simple, interpretable, and effective for linear relationships but struggled with complex, nonlinear interactions and required manual preprocessing where AI models excel.[116] Deep learning now captures nonlinear relationships and automates feature extraction, outperforming traditional methods in accuracy and robustness. Despite these advantages, AI models can be prone to overfitting, and require careful validation, whereas traditional methods remain useful for smaller data sets and scenarios where explainability is crucial.[121]

Gas sensors produce signals in a variety of forms, with many of those signals falling into two categories: time-series signals, such as that produced by a single MOS gas sensor, and spectral signals, as produced by direct absorption spectroscopy gas sensors; see Figure 4 for examples of these two types. While

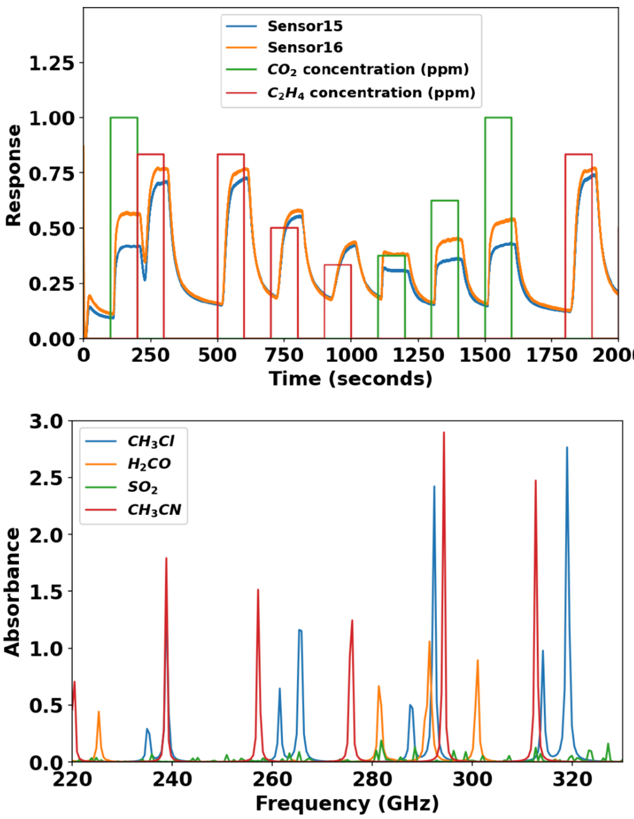

Figure 4. Top: example MOS time series data;[122] bottom: example spectral absorption data for gas sensing using rotational spectroscopy.[127]

these time-series and spectral data are 1-D in their simplest forms, many sensors and signal processing systems produce 2-D, 3-D, or higher-dimensional data. For example, spectral data can be represented in 2-D using Gramian methods, in 2-D for time-resolved spectra, or in 2-D, 3-D, or 4-D for time-resolved tomographic measurement systems.

The volume and type of data generated depend significantly on the individual experimental setup and objectives. For instance, in gas sensing applications, data such as time series responses from MOS sensors or spectral absorption profiles from rotational spectroscopy are typically collected over varying concentrations of target analytes.[54,122−125] Experimentalists often generate extensive data sets by varying environmental conditions, such as temperature, pressure, or interference from other compounds, to ensure robustness and generalizability of the ML models.[126] Input data

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Table 1. Overview of Common Machine Learning, Deep Learning, and AI Methods for Gas Detection and Quantification

Method	Description
Linear Discriminant Analysis	A classification method that finds a linear combination of features to separate classes (e.g., gases, combination of gases) by maximizing the ratio of between-class variance to within-class variance.
Quadratic Discriminant Analysis	An extension of LDA which allows each class to have its own covariance matrix, enabling the decision boundaries to be quadratic rather than linear.
Ridge Regression	Applies L2 regularization to linear regression to control the complexity of the model by penalizing large coefficients to obtain a simpler model.
Lasso Regression	Applies L1 regularization to linear regression, allowing some coefficients to shrink to zero for feature selection.
Logistic Regression	Classifies inputs by applying the logistic function to a weighted sum of the features, modeling the probability of the categories of gases.
Support Vector Machine	Seeks an optimal boundary that separates classes of gases by maximizing the margin between them.
Support Vector Regression	Uses the margin concept from SVM to minimize prediction errors for continuous outputs.
Decision Trees	Repeatedly splits data based on feature thresholds, forming a hierarchical set of if–then rules for gas detection or concentration quantification.
Ensemble Methods	Includes bagging (e.g., Random Forests), boosting (e.g., Gradient Boosting, AdaBoost, XGBoost), and stacking, which combines outputs of base models through a meta-learner.
Random Forest	Creates an ensemble of decision trees to aggregate predictions and reduce variance.
K-Nearest Neighbors	Classifies or regresses a point based on the majority vote or average among its closest neighbors.
Neural Networks	Learns complex patterns by passing inputs through interconnected layers of weighted nodes.
Deep Learning	Extends neural networks with multiple hidden layers to capture more intricate feature representations.

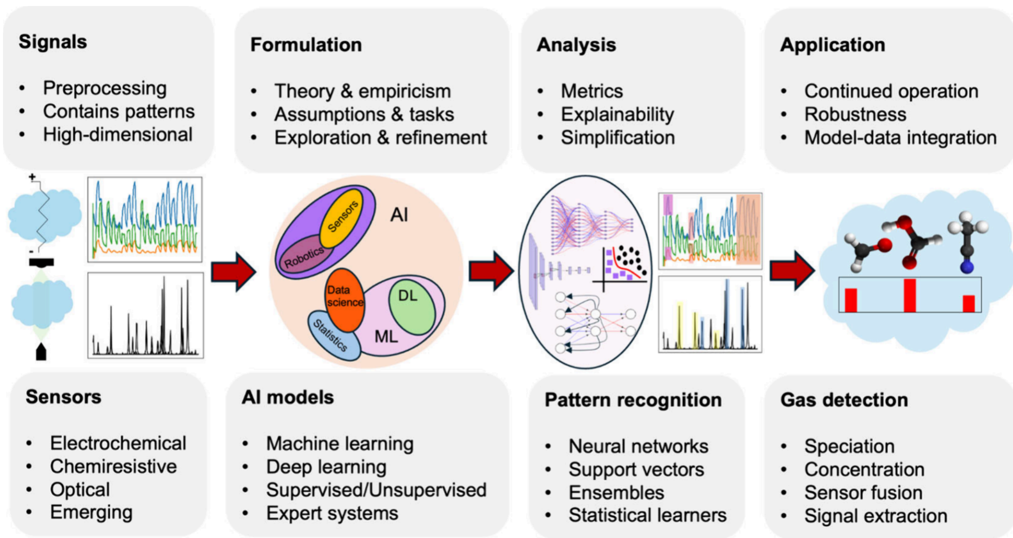

Figure 5. Workflow for AI integration in gas sensing.

segmentation involves splitting the data set into training, validation, and testing sets, usually ensuring that each subset covers the diversity of experimental conditions.[52]

Numerous AI methods exist for feature extraction, classification, and data interpretation that can be applied to gas sensing. However, before the implementation of AI-based methods, sensor signals are typically processed by using non-AI methods. For example, sensor signal processing can include baseline correction, drift correction, amplitude normalization, cropping, time alignment, segmentation, smoothing, and filtering. Implementing these preprocessing steps ensures that sensor data has high signal-to-noise, is consistent, and is optimally prepared for AI, ML, or DL methods.

Rather than review the significant developments in AI, ML, and DL methods that have taken place over the last several decades, we will point the reader to recent reviews and texts on AI by Hopgood,[128] Bishop,[129] and Wang et al.[130] and ML and DL by Alpaydin,[131] Murphy,[132] Roberts,[133] Goodfellow et al.,[8] and Zhang et al.[134] Supervised learning has been widely implemented in gas sensing and significantly more than unsupervised and reinforcement learning. However, unsupervised methods, k-means clustering, hierarchical clustering, and self-organizing maps (SOMs) have been used to identify patterns in sensor signals without requiring labeled data.[16] Unsupervised algorithms, including principal component analysis (PCA), have been used to identify sensor outliers or faults.[135] PCA and t-distributed stochastic neighbor embedding (t-SNE) have been used to reduce the dimensionality of gas sensor data.[16]

Supervised learning methods have been widely applied in gas sensing, with many examples described in the section "Application of AI to Gas Sensing". These methods can be categorized into classification, regression, ensemble, dimensionality reduction, anomaly detection, and time series forecasting methods. Standard ML classification methods have been widely used for pattern recognition in gas sensor signals for gas detection including logistic regression classifiers (LRCs), support vector machines (SVMs), decision trees (DTs), random forest (RF), k-nearest neighbors (kNNs), neural networks (NNs), and DL methods. Standard ML

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regression methods have also been used for quantitative gas concentration determinations, including linear, polynomial, ridge, and lasso regression, support vector regression (SVR), and DT and NN regression. Ensemble methods have also been applied for classification and regression, including bagging (e.g., RF), boosting (e.g., gradient boosting, AdaBoost, and XGBoost), and stacking.

While we recommend the references cited above for descriptions of ML, DL, and AI methods, Table 1 summarizes some popular methods.

DL methods, including DNNs and convolutional neural networks (CNNs), have been widely applied to classification and regression in gas sensing applications. Gas sensor time-series data have been treated with DL methods, including recurrent neural networks (RNNs), long short-term memory (LSTM), and gated recurrent units (GRUs). Autoencoders have been used in gas sensing for feature extraction, dimensionality reduction, and anomaly detection. The Application of AI to Gas Sensing section reviews the application of these and other AI methods to gas sensing.

Figure 5 outlines a workflow for AI model development and implementation in gas sensing. Measured signals from gas sensors or sensor arrays contain identifiable latent patterns that allow for a sensing task or application, such as speciation, concentration prediction, signal extraction (denoising or low-dimensional representation), or sensor data fusion. These applications can be carried out from sensor signal patterns identified using AI and through the analysis of AI formulations and the signals themselves. Thus, developing an AI model for a particular sensor is initiated by formulating these assumptions and hypotheses, which are collected together. Specific protocols vary across studies; a general workflow involves systematic data collection, cleaning, and annotation (for classification), followed by exploratory analysis to understand the patterns and outliers before feeding the data into ML pipelines. Reliable AI models are the product of the crucial interplay between experimental rigor and computational methodologies.

The sensing framework can also be combined with a theoretical understanding of the sensing task. For example, simulations based on theory can be used to train the model. Furthermore, any empirical knowledge can be injected into the model development process, such as any compensation algorithm to boost the sensor data, address dynamic offsets, etc. At this point, an AI model can be developed to process the assumptions, hypotheses, theory, and empirical adjustments and can be applied to recognize patterns in sensor signals. The user may want to explore different AI models to suit their needs; hence, the exploration of models and their unique pattern recognition capabilities is typical.

Following some level of AI model development, the developer may decide to finalize the model for sensor operation, or further model simplifications can be made. In this sense, model development and application are an iterative, cyclical process. For example, the developer may realize that only part of the data stream is necessary, recognition of only part of a pattern is required, the quantity of training data can be reduced, or features can be eliminated. Model simplification can be done by redefining the assumptions and hypotheses embedded in the model. Throughout the iterative model development, the developer often gains an improved understanding of how the model and environmental parameters affect the AI performance and the physics or chemistry that governs the sensor−AI system. Such a renewed understanding may allow the AI model to be developed further. The developer can also use a variety of methods to interpret the model and the model data integration process, such as local interpretable model-agnostic explanation (LIME),[136] Shapley additive explanations (SHAP),[137] or gradient-weighted class activation mapping (GradCAM).[138]

■ APPLICATION OF AI TO GAS SENSING

Smart gas sensing technology integrates AI into the gas sensor technologies described in the Gas Sensing Methods and Technologies section, automating their operation and enhancing the sensor performance. Key components of these technologies include the gas sensor or sensor array, signal processing techniques that mitigate drift and other signal aberrations while providing feature extraction, and algorithms that enable gas pattern recognition and quantitative concentration measurement. Sensor arrays or multisensor configurations can offer advantages by leveraging the complementary strengths of individual sensors to address common challenges in gas sensing, such as cross-sensitivity and selectivity. Additionally, smart gas sensing can employ "brain-like" AI methods to enhance sensitivity and decision-making, thereby improving the analysis and interpretation of signals from gas sensors.[15] As discussed in this section, established ML and DL models have demonstrated exceptional performance in gas classification and quantification utilizing a broad array of sensing methods.

AI-Based Electrochemical Gas Sensors. Recent advancements in integrating AI and ML into electrochemical gas sensors have shown potential for enhancing sensor performance, accuracy, and reliability for environmental monitoring and industrial applications; see Table 2 for several examples. One of the primary challenges in electrochemical gas sensors is sensor drift, which can affect the accuracy of long-term measurements. Recent studies have demonstrated that AI/ML algorithms, such as RF regressors and LSTM networks, can effectively address this issue. For instance, Han et al. applied these algorithms to calibrate low-cost sensors for gases like NO_2, O_3, and CO, substantially improving measurement accuracy.[139]

Another area where AI/ML integration with electrochemical gas sensors has made strides is the pattern recognition and classification of gas mixtures. By employing DL models, sensors can detect the presence of specific gases and classify complex mixtures with high accuracy. For example, Smith et al. have applied a variety of ML methods, including logistic and Bayesian regression, boosted regression trees, Gaussian processes, and CNNs, to classify NO_2, O_3, CO, and various VOCs using data from electrochemical sensors, achieving high classification accuracy even under challenging environmental conditions.[140,141]

Adaptive learning models have been increasingly used to allow electrochemical sensors to perform reliably in dynamic environments. These models continuously learn and update their parameters in real-time based on new data, improving the sensor's response to temperature, humidity, and other environmental factors. This approach was effectively demonstrated by Ma et al.,[142] who integrated an electrochemical sensor array with RK, NN, and kNN methods to monitor methane concentrations, achieving over 98% accuracy despite significant environmental variability.

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Table 2. Examples of Integrated AI–Gas Sensor Systems[a]

Sensor System	Type of AI	Gases	Application	ref
Electrochemical Sensors				
Custom electrochemical	SLR, BLR, BRT, GPR	NO_2, O_3, CO, VOCs	RGN	141
Commercial electrochemical	SVM	NO_2, O_2	CLF, RGN	191
Electrochemical	LRC, SVM, RF, NBC, k-NN	CH_4, NH_3, natural gas	CLF	142
Electrochemical	SLR, MLP, RF, LSTM	CO, NO_2, O_3, and SO_2	CLF, RGN	139
Chemiresistive MOS Sensors				
MOS	GRU, t-SNE, DNN	H_2	CLF	54
MOS array	SVM	C_2H_4, CO	CLF	45
MOS	RNN, CNN	NO_2, H_2S	RGN	151
MOS array, thermal camera	LSTM, CNN	CO, CH_4, butane, LPG, alcohol, smoke, natural gas	CLF	152
MOS	RF, MLP, SVM	Formaldehyde, methanol, propanol, toluene	CLF	192
MOS	SVM, SVM	CO, O_3, NO_2	CLF	143
MOS	CNN	CO, NH_3, NO_2, CH_4, acetone	CLF	144
MOS array	PCA, ANN, DNN, 1-D CNN	Benzene, toluene, xylenes, ethanol, formaldehyde	CLF	145
MOS array	MCNA, SVM, RVM, MLP, LSTM, CNN	Acetaldehyde, acetone, benzene, butanol, ethylene, methanol, toluene, CO, CH_4, NH_3	CLF	146
MOS array	MLP, CNN, RNN	CO, CH_4, ethylene	RGN	156
Commercial MOS array	DNN	CO, ethylene	CLF	123
MOS array	DNNs and CNNs (tuned GoogLeNet, ResNet, AlexNet)	CH_4, CO, ethylene, ethanol	CLF	155
Nanowire sensor	CatBoost, XGBoost, LightGBM, Extra Tree	Ethanol, propanol, butanol, hexanol, acetone, acetic acid	CLF	193
MOS, electrochemical, photoionization	NN	Acetone, propane, butane, benzene, carbon tetrachloride, trimethylphosphite, ethylene, ethylene oxide, hydrazine, hydrogen peroxide, CH_4, Cl_2, H_2S, H_2, NH_3, NO_2, O_2	CLF	148
MOS array	1-D CNN	Formaldehyde, toluene, NH_3 and their mixtures	CLF	149
MOS array	k-NN, DT, SLR, LRC, NBC, LDA, NN, SVM	Phenol, acetone, toluene, chloroform	CLF, RGN	150
Nanoparticle Decorated (ND) MOS Sensors				
ND MOS	DNN, RF, SVM, NBC	Acetone, benzene, ethanol, formaldehyde, methanol, propanol, toluene	CLF	63
ND MOS	PCA, CNN	CO, NO_2, NH_3, and their mixtures	CLF	65
ND MOS	DNN	Acetone, benzene, ethanol, formaldehyde, methanol, propanol, and toluene	CLF	64
ND MOS	PCA, LDA, LRC, NN, MLP	Acetone, ethanol, methanol, toluene	CLF	66
E-Nose Sensors				
MOS array E-Nose	SVM, MLP, 2-D CNN (GasNet)	CO, CH_4, H_2, C_2H_4	CLF	24
MOS array E-Nose	1-D LSTM, CNN, k-NN, SVM, RF	Trinitrotoluene (TNT)	CLF	164
MOS array E-Nose	k-NN, SVM, 2-D CNN (GasNet, ResNet), MLP	Acetone, acetaldehyde, butanol, ethylene, methanol, benzene, toluene, NH_3, CH_4, CO	CLF	173
MOS array E-Nose	SVM	Ethylene, CO	CLF	45
MOS array E-Nose	LSTM, LDA, NBC, SVM, k-NN, ensemble methods	Ethylene, ethanol, CO, CH_4	CLF, RGN	165
MOS array E-Nose	k-means, NN, CNN	NO_2, CO, and mixtures	CLF	167
Commercial MOS array E-Nose	DNN, SVR	Ethanol, methanol, isopropanol, pentane, hexane, furan, butyric acid, acetaldehyde, and mixtures	CLF, RGN	168
MOS array E-Nose	1-D CNN, DBN	Ethylene, CO, CH_4, and mixtures	CLF, RGN	194
MOS array E-Nose	CLSTM, MLP, SVM	Propane, CO, CH_4	CLF	170
MOS array E-Nose	CNN, SVM, NN, ensemble methods	Butanol, xylenes, acetone, acetaldehyde, ethylene, ethanol, toluene, NH_3	CLF	179

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Table 2. continued

Sensor System	Type of AI	Gases	Application	ref
E-Nose Sensors				
Electromechanical/MEMS or transduction based	PCA, LDA, QDA, SVM, k-NN	He, Ar, CO_2	CLF	186
MOS array E-Nose	CNN	Wide variety of gases	CLF	169
MOS array E-Nose, thermal images	CNN, Bi-LSTM, DWT, DCT with fusion approaches	Smoke ($CO + NO_2 + CO_2 + SO_2$), mixtures, perfumes	CLF	180
MOS array E-Nose	DNN	Methanol, ethanol, acetone, NO_2	CLF, RGN	195
MOS array E-Nose (Fonollosa 2015)	CNN, MLP, SVM	Ethylene, CH_4, and mixtures	CLF, RGN	176
MOS array E-Nose (Fonollosa 2015)	CNNs (tuned GoogLeNet, ResNet, AlexNet)	Ethanol, ethylene, CH_4, CO	CLF	155, 122
MOS array E-Nose	CNNs	Wide variety of gases	CLF	53
MOS-Array (EN)	1-D CNN	Formaldehyde, toluene, NH_3 and their mixtures	CLF	149
Olfactory EEG Commercial MOS array E-Nose	NNs			171
MOS array E-Nose	1-D CAE, 1-D CNN with ArcLoss	CH_4, and oils and coffee	CLF	172
Graphene-based E-Nose	LDA, PCA	NO_2	CLF	166
Graphene-based E-Nose	PCA, LDA	Ammonia, acetone, ethanol, 2-propanol, sodium hypochlorite and water vapor	CLF	163
Graphene-based E-Nose	PCA, RF	Ethanol, hexanal, methyl ethyl ketone, toluene and octane	CLF	77
Graphene-based E-Nose	SVM, 1-D CNN, RF-based	NH_3, NO, NO_2 and H_2S molecules	CLF	78
Graphene-based E-Nose	PCA, XGBoost	Methanol, 1-propanol, 2-propanol, 2-butanol, 1-butanol, and ethanol	CLF, RGN	161
CNT-Based	Several potential ML methods in CNT-ML application	Several gases including CO_2, HCHO, acetone and NO	CLF, RGN	69, 72, 74
MOS with MoS_2 nanoflakes with defects and exposed-edge sites	PCA, kNN, NN, SVM, LDA	Triethyleamine, nonpolar VOCs	CLF	84
TM-WSe_2-based	RF, GBR, EGB, SVR, KNN, MLP, KRR, GPR, DT, and ET	N_2O, CH_4, SF_6, CO_2	CLF	85
Optical Sensors				
Optical, IR	PCA, LRC, RF, SVM, SLR, NN	Water vapor	RGN	94
Optical, IR	1-D CNN, DNN, DT, ABDT, k-NN	CH_4, acetylene	RGN	96
Optical, THz	1-D CNN	Acetaldehyde, acetonitrile, chloromethane, methanol, ethanol, formic acid, nitric acid, formaldehyde, HCN, H_2S, SO_2, OCS	CLF	127
Optical, IR	CNN	CO, CH_4	RGN	95
Optical, THz	1-D CNN	Acetaldehyde, acetonitrile, chloromethane, methanol, ethanol, formic acid, nitric acid, formaldehyde and their mixtures	CLF	119
Optical, IR	CNN	H_2O, CO_2, O_3, N_2O, CO, CH_4, NO, SO_2, NO_2, NH_3	CLF	175
Optical, IR	SVM, NN	CO, CO_2	RGN	183
Optical, UV	2-D CNN	Benzene, toluene, ethylbenzene, xylenes	CLF, RGN	97
Optical, IR	MLP, k-NN, SVM	CO_2, CH_4	CLF, RGN	184
Liquid Crystal Sensors				
Liquid crystal	2-D and 3-D CNN, LSTM	Acetone, acetonitrile, chloroform, dichloromethane, diethyl ether, butyric acid, hexane, heptane, methanol, toluene	CLF, RGN	107
Liquid crystal	3-D CNN	O_3, Cl_2	CLF	108
Emerging Sensor Types				
MEMS	PCA, LDA, QDA, SVM, k-NN	He, Ar, CO_2	CLF	186
Ultrasonic Time of Flight	NN, CNN	Air and Ar in He	RGN	185

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Table 2. continued

Sensor System	Type of AI	Gases	Application	ref
Emerging Sensor Types				
Perovskite sensors	CNN, MLP, RF, LRC, DT, SVM, Bagging, Voting	Ethylene, benzene, dimethyl ether, methyl formate, ethanol, methanol, HF, CO_2, CO, H_2, CH_4	CLF	36
SAW	SVM, RF	Toxic gases	CLF, RGN	187−189
QCM	NN	SO_2	RGN	190

[a]See List of Acronyms for the AI method abbreviations. CLF: classification or species detection; RGN: regression task or concentration prediction.

The use of AI in managing data from multiple electrochemical sensors has also gained traction. By leveraging the complementary strengths of different electrochemical gas sensors, AI algorithms can optimize data fusion processes, improving the overall system performance. For example, Smith et al. explored using AI-driven multielectrochemical sensor systems to address issues like cross-sensitivity and selectivity, resulting in more robust and reliable gas detection systems.[141]

AI-Based Chemiresistive MOS Gas Sensors. The incorporation of ML models has mitigated the limitations of chemiresistive MOS gas sensors including poor selectivity and drift issues when dealing with complex gas mixtures. ML models benefit from the detailed feature data extracted from chemiresistive sensors, making them adept at distinguishing between similar gas responses and overcoming the fundamental weakness of traditional chemical sensors. The combination of MOS gas sensors and ML or DL allows for the extraction of temporal features and relationships among different signals, outperforming traditional methods in terms of efficiency and accuracy. See Table 2 for many exemplar demonstrations of MOS-based chemiresistive gas sensing that AI has enhanced, automated, or otherwise improved.

Djeziri et al. demonstrated a MOS sensor enhancement using a temporal-based SVM for the detection and identification of multiple toxic gases in mixtures, specifically targeting gases such as NO_2, O_3, and CO.[143] Their method employs an incremental algorithm to optimize the selection of kernel functions, aiming to balance accuracy with simplicity in implementation. The methodology is further enhanced by a decision-making algorithm that analyzes the appearance rate of gases within a moving window, effectively managing uncertainties and improving the reliability of decisions. This algorithm is crucial for reducing false positives and nondetections, providing quantifiable confidence in the system's outputs. Experimental results underscore the effectiveness of this approach, which achieved 100% accuracy in both the learning and testing phases, even in challenging, noisy environments.[143] Bae et al.[45] have also investigated the selectivity for a target gas and the accuracy of concentration measurements for MOS sensor signals processed via an SVM model.

Several investigators have integrated MOS sensors with CNNs. For example, Kang et al.[144] have fabricated uniform arrays of nanocolumnar films of SnO_2, In_2O_3, WO_3, and CuO MOS gas sensors and integrated them with a CNN for real-time selective detection of CO, NH_3, NO_2, CH_4, and acetone. This approach achieved high detection accuracy and rapid response times, demonstrating significant improvements in the practical application of MOS gas sensors for environmental monitoring.

Oh et al.[145] have successfully used 1-D CNNs and DNNs to discriminate indoor pollutants, even in environmental variations. Specifically, five VOCs, benzene, xylene, toluene, formaldehyde, and ethanol, were detected and discriminated using a sensor array of five In_2O_3-based MOS gas sensors. Predictions utilizing DNNs proved more effective than 1-D CNNs for training, validation, and test data sets, and it was determined that ML methods were more effective at gas discrimination under temperature and humidity fluctuations relative to traditional methods.[145]

Pan et al.[146] have developed a multiscale CNN with attention (MCNA). This lightweight network integrates a multiscale deep CNN with a self-aware mechanism for

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identifying ambient gases using MOS gas sensor arrays. MCNA can offer superior generalization and identification accuracy under varying operating conditions. The MCNA incorporates a self-aware mechanism to enhance feature extraction, resulting in a more robust and generalizable model. Their MCNA exhibited superior performance, particularly in generalization and efficiency.[146]

A significant challenge for detecting multiple gases in mixed environments is time-series sensor data processing techniques that can complement DL models. Multitask learning, which leverages the mixed-gas nature, provides synergistic benefits, including incorporating on−off classification as part of the hybrid learning task. When sensors with time series responses are integrated with models, such as multilayer perceptrons (MLPs), CNNs, and RNNs, CNNs generally outperform other models when analyzed jointly with the learning task. This is demonstrated using the University of California Irvine gas mixture data set,[122] featuring 16 sensors exposed to C_2H_4, CO, and CH_4 gases. The results demonstrate significant improvements in estimation accuracy over previous studies, highlighting the effectiveness of the joint learning task-based approach.[147]

Ku et al.[148] have demonstrated that the integration and optimization of MOS gas sensors with other sensor types using artificial neural networks (ANNs), DNNs, and 1-D CNNs can result in a high-performance, compact, and efficient system for identifying and preventing hazardous gas leaks with minimal gas sensing data. In this demonstration, implementing ML/DL methods allowed even single-mode MOS gas sensors to perform well due to their inherent cross-sensitivity, which is typically considered a drawback. An optimized ML strategy based on multisensor inputs and focusing on sensor transients allowed sensor performance improvements relative to standard methods.[148]

Mu et al.[149] developed a MOS micro-electromechanical system (MEMS) gas sensor array made of ZnO, SnO_2, and CNT materials. The array was prepared by inkjet printing onto a micro-hot-plate. A 1-D CNN was employed to identify seven gases, achieving high recognition accuracy for variable time series input lengths (sampling times). Similarly, Singh et al.[150] reported a MOS sensor array composed of NiO−Au, CuO−Au, and ZnO−Au sensors fabricated using the DC reactive sputtering method, exhibiting high cross-sensitivity. They applied their MOS array to detecting VOCs in human breath to enable early, noninvasive disease diagnosis. Their work leveraged various ML methods (RF, k-NN, DT, LRC, NBC, LDA, ANN, and SVM) to identify and quantify ethanol, acetone, toluene, and chloroform individually and in mixtures.

Jaleel et al.[123] reported a classification system for gas detection based on MOS gas sensors using both 1-D time series data and 2-D Gramian angular field (GAF) data, a pictorial transformation of a time series suitable for CNNs. Signals from the MOS array were input as 1-D time series data to an improved version of GasNet[24] and in the form of 2-D GAF images to the AlexNet model[6] to provide superior classification performance for gas detection.

RNNs and LSTM, designed to process sequential data, were implemented to process time-series MOS sensor signals. For example, Kwon et al.[151] implemented RNNs for processing signals from In_2O_3 film MOS gas sensors to detect NO_2 and H_2S. LSTM was implemented by Narkhede et al.[152] to process a MOS gas sensor array composed of seven semiconductor sensors that detect CO, NO_2, and CH_4. They also combined the sensor data with thermal images processed by using CNNs in a hybrid sensor fusion modality.

DNNs have been widely applied for gas recognition based on MOS gas sensors. MOS data encoded into 2-D images using the GAF method improved the robustness and generalization in the DNN processing of MOS signals. Combining this preprocessing with the fine-tuning of the GoogLeNet network,[153] Wang et al.[155] demonstrated excellent classification of four gases from MOS sensors: methane, ethanol, ethylene, and carbon monoxide. Their proposed gas recognition network outperformed other models like fine-tuned ResNet50 and ResNet34[154] and AlexNet[6] for both accuracy and sample processing times.[155]

The discriminative information is often buried in noise within a signal, resulting in poor signal-to-noise ratios. Given sufficient data, DNNs can learn unique patterns for detecting gas molecules. Cho et al. have applied DNNs to detect “hidden signals” in noisy data beyond the limits of detection from MOS gas sensors for hydrogen gas across multiple different metals, demonstrating improved sensitivity and specificity that were previously unachievable. This approach revealed discriminative low-dimensional representations in frequency and time domains, shedding light on relative similarities and dissimilarities among signals.[54]

A CNN model, augmented with ResNet18[154] and additional layers, was developed by Eo et al. for MOS-based detection of ethylene, CO, and methane.[156] Their DL framework was tailored for predicting concentrations in mixed-gas environments and focused on synergistic approaches in data preprocessing, network architectural decisions, and multitask learning. The roles of various preprocessing techniques, such as data cleansing, reduction, noise reduction, normalization, and lag correction, were explored, and normalization and lag correction were identified as effective methods for improving model performance. A mixed-gas detection and concentration estimation framework, using multitask learning and different DNN architectures (MLP, CNN, and RNN), was compared after applying these preprocessing techniques. When augmented with ResNet18[154] and additional layers, the CNN model outperformed the others.[156]

AI-Based Nanoparticle-Decorated MOS Gas Sensors. The accuracy and selective detection of VOCs using nanoparticle-decorated MOS sensors and sensor arrays coupled with ML methods have been reported in recent literature. Acharyya et al. used a sensor array consisting of four separate sensing layers over interdigitated electrodes, each decorated with silver, gold, palladium, and platinum nanoparticles, for the sensitive sensing of CO_2, NO_2, CO, and O_2. Their nanoparticle-decorated MOS sensor array was integrated with a DNN, with a time series sequence as input, to provide quantitative detection of VOCs. The system achieved superior classification accuracy relative to traditional MOS signal processing methods and fast prediction times.[63] In further work by Acharyya et al., a stand-alone MOS gas sensor system with wireless monitoring and Internet connectivity, fabricated using platinum-decorated tin-oxide hollow spheres as the sensing material, effectively detected acetone, benzene, ethanol, formaldehyde, methanol, propanol, and toluene at various concentrations using a DNN.[64]

Kim et al. reported MOS gas sensors based on indium oxide (In_2O_3), tin oxide (SnO_2), and titanium dioxide (TiO_2), designed to enhance selectivity by using composites of these metal oxides and decorating them with catalytic gold nanoparticles. These sensors effectively detected CO, NO_2, and NH_3 at various concentrations. Kim et al. employed a CNN model to differentiate these gases and their mixtures based on sensor response, achieving excellent discrimination and efficiency.[65]

Somalapura Prakasha et al. produced a MOS gas sensor with a sputtered ZnO thin film loaded with Au nanoparticles that is highly sensitive to acetone, ethanol, methanol, and toluene. Multiple sensors with different Au loadings address cross-sensitivity issues, and ML algorithms enhanced discriminative analysis.[66]

AI-Based Electronic Nose. An electronic nose (E-nose) sensor system detects gases (odors) by mimicking the human olfactory system. It consists of many sensors in an array, typically but not exclusively chemiresistive MOS gas sensors, each sensitive to a different gas or category. When an E-nose array interacts with gases of interest, it generates a unique pattern of responses that can be analyzed by using AI or ML algorithms to specifically identify a gas or mixture of gases.

Although many E-nose configurations depend on commercial chemiresistive MOS sensors,[157−160] emerging gas sensing platforms employing graphene, CNTs, transition metal dichalcogenides (TMDs), and other non-MOS-based materials are rapidly shaping modern E-nose designs.[77,161−163] Important applications include VOC or odor detection, food and beverage quality monitoring, medical diagnosis and disease detection, and explosive detection, among other security and defense applications,[164] where accurate gas concentration measurements and selective gas detection are crucial. E-noses typically comprise a sensor array, an electronic signal processing system, and an AI-based pattern recognition algorithm. Ultimately, an E-nose's signal processing and pattern recognition components involve several key steps: preprocessing, feature extraction, classification, and regression.[165] While traditional approaches to gas identification using MOS gas sensors have focused on single gas detection, limiting their applicability to scenarios involving gas mixtures, E-noses can address mixtures by combining feature extraction and pattern recognition. A recent study on a graphene-based e-nose functionalized with diazonium chemistry for effective nitrogen dioxide detection and discrimination among interfering gases demonstrated high sensitivity and prediction accuracy using LDA and PCA based models, proving its potential for environmental monitoring, safety, and medical applications.[166] Many studies have been reported in the literature on E-nose gas detection enabled by AI-based signal processing, feature extraction, and pattern recognition;[167−170] see Table 2 for several recent studies on AI in E-nose systems.

E-noses are known for artificial sensory evaluations, such as odor recognition. The odor recognition problem is complicated due to poor repeatability and the inability of machines, such as the E-nose, to capture the emotional and subjective nuances of human odor preference. Integrating physicochemical odor data with personal sensory responses requires a methodology involving a reliable and robust data acquisition and preprocessing protocol for both the olfactory electroencephalogram (EEG) (the brain's response to smell) and gas sensors coupled with a complementary data mining strategy focusing on extracting both individual and common features from the multimodal data, thus enabling the system to recognize and generalize across olfactory preferences.

By leveraging CNNs, improved E-noses have been proposed with powerful data mining capabilities, enabling more effective feature extraction and classification than traditional ML methods and showcasing the handling of cross-subject variability in nuanced odor recognition. Smart E-noses from cutting-edge gas sensors integrated with state-of-the-art DL methods can narrow the divide between human sensory evaluation and machine-based measurement.[171] Feature extraction via a 1-D convolutional autoencoder (1D-CAE) and a 1D-CNN integrated with customized loss functions have shown great promise in further enhancing E-nose capabilities.[172] Real-time detection in embedded E-noses has been reported with a lightweight, high-precision CNN called SeparateNet, along with a novel data transformation method named dislocation-stack that achieved excellent performance metrics on 14 electronic nose data sets.[53]

CNNs allow for feature maps capturing discriminative gas information generated from E-nose signals. Such feature maps can be combined with image-handling neural networks to achieve superior classification accuracies.[173] Effective feature extraction ensures that robust pattern information is retained while removing noise and redundancy from raw signals. Effective downstream ML methods can then be used for accurate gas predictions. Feature extraction from E-nose data can also be effectively performed by using LSTM networks. These networks have successfully classified and regressed tasks when SVM processes the extracted features for classification and Gaussian Process Regression (GPR) for regression tasks.[53] Additionally, Bakiler and Güney[165] showed that the combination of LSTM networks with discrete wavelet transform (DWT) can surpass traditional methods like k-NN, linear discriminant analysis (LDA), and SVM/SVR in tasks that involve noisy time-series data, such as predicting concentrations.[165]

Classical methods (MLP, PCA, k-NN, SVM, DT, neural basis model (NBM), and LDA) are typically effective when features are selected correctly, particularly for mixtures containing a limited number of target gases. However, these classical methods have relatively fixed frameworks and few parameters and typically struggle with multigas recognition under noisy conditions[174] where DNNs have excelled.[24,52,54,119,127,175,176] In contrast, DNNs contain many more parameters and can learn and adapt to the complex features of gas sensor data, reducing the need for manual feature extraction and improving accuracy. DNNs transform input space through multilayer nonlinear transformations, making data classes (gas types) linearly separable. This capability allows for automatic learning of deep-level gas characteristics, enhancing the performance and universality of the E-nose systems. Data preprocessing techniques, such as wavelet filters, Kalman filters, and Savitzky−Golay filters, to remove noise and standardize data further assist the predictive DNN models by producing better features.[177]

Despite significant advancements in sensor materials, certain challenges persist in enhancing the gas sensor performance arising from environmental factors as well as sensor aging and contamination.[15] Additionally, differentiating gases in mixed scenarios remains difficult due to sensor cross-reactivity.[178] Sensor drift is often caused by variable environmental conditions such as temperature, humidity, air pressure, and factors such as sensor aging and contamination. Drift compensation is required to address the degradation of sensor accuracy due to drift.[17] Augmented CNNs have been proposed as a continuously updated ML framework designed to solve gas discrimination problems over extended periods where drift is

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present. The augmented CNN model transforms time-varying gas signals into a multidimensional feature matrix and uses incremental data to extend the model's knowledge through internal parameter tuning and counteract the degrading effects over short-term self-collected data (4 months) to a long-term public data set (3 years).[179] The cross-reactivity problem for E-noses poses a challenge that can be addressed via hybridized multimodal sensors, combining chemiresistive MOS gas sensor arrays with other sensor types (e.g., optical, electrochemical, etc.). For example, a DL-based sensor system that combines multimodal data from IR thermal imaging and an array of seven MOS sensors utilizes three CNNs for feature extraction and bidirectional long short-term memory (Bi-LSTM) for gas detection was reported by Atallah.[180] Attallah also explored methods for multimodal data fusion to enhance gas detection.[180] Recent studies reported improvements in long-term stability and mixture speciation, utilizing an E-nose in chemiresistive and FET configurations.[78,166]

AI-Based Optical Gas Sensing. Optical gas sensing methods often rely on detecting a spectral feature or signal, such as an absorption feature, due to quantized electronic, vibrational, or rotational transitions. AI methods can classify the gas identity based on observed features and provide quantitative gas concentrations; see Table 2 for several examples. AI models can be trained with analytical or synthetic data derived from theoretical, computational, or experimental approaches to achieve superior selectivity and predictive capabilities. This strategy has been particularly effective in optical gas sensing. For example, Chowdhury et al. have demonstrated the application of ML and DL models to spectral classification and gas detection based on direct absorption spectroscopy within the THz (rotational transitions) and IR (vibrational transitions) regions.[52,119,127,175,181] The true potential of ML and DL models is realized in their ability to selectively classify gases in complex mixtures where traditional methods are often not effective.[119,175] In recent work, DNNs have emerged as particularly successful among models for gas classification when integrated with optical gas sensors due to their advanced feature engineering capabilities, scalability, explainability, and ease of integration, allowing the development of optical sensors that achieve high responsivity and excellent chemical specificity.[182]

Tunable direct laser absorption spectroscopy (TDLAS), a widely developed gas sensing method that integrates the rovibrational spectra of gases, is advantageous for high-fidelity gas sensor systems due to the molecular fingerprints provided by IR absorption features. However, TDLAS has often been limited to the laboratory, and there are difficulties associated with its implementation in applications due to limitations arising from baseline fitting, background noise, and signal drift. A TDLAS gas sensing system using end-to-end 1-D CNNs was explored for accurately measuring and detecting gases and providing concentrations. For example, Tian et al. developed TDLAS systems coupled to CNN signal processing to detect methane and acetylene, with the potential for reliable application to many other gas molecules.[96]

Separating overlapping absorption features is crucial for the simultaneous classification and quantification of multiple gas components from the absorption spectra. However, DL models for identifying multicomponent gas mixtures from IR absorption spectra remain largely underexplored. Recently, Chowdhury and Oehlschlaeger reported a 1-D CNN-based model, trained on HITRAN-based simulations, to detect small molecules from their IR absorption spectra in flexible, user-defined frequency ranges. Their model achieves excellent classification accuracy for many target molecules, including water vapor, carbon dioxide, ozone, nitrous oxide, carbon monoxide, methane, nitric oxide, sulfur dioxide, nitrogen dioxide, and ammonia, gases relevant to atmospheric, industrial, and environmental processes.[175]

Sun et al. reported a gas sensor for detecting carbon monoxide (CO) and methane (CH_4) based on TDLAS and one-dimensional CNNs trained, tuned, and tested on simulated data. ML-based sensing systems successfully overcame the spectral cross-interference problems that stem from many overlapping spectral lines.[95] Guan et al. reported cavity-enhanced direct frequency comb spectroscopy integrated with several ML models for high-fidelity gas concentration measurements. Their work showed that the particle swarm optimization SVM model achieved high predictive accuracy and enabled increased sensor compactness and suitability for outdoor applications.[183] Sun et al. developed a stepwise MLP algorithm for the rapid and accurate detection of gas mixtures, focusing on the detection of CO_2 and CH_4 from NDIR spectroscopy signals.[184]

AI-Based Liquid Crystal Gas Sensors. Frazão et al. demonstrated quantitative VOC gas sensing using liquid crystal (LC) droplets in hybrid gels assisted by a CNN-based algorithm. Their CNN-based method enables the extraction of rich feature information originating from variations in the optical texture dynamics recorded by using polarized optical microscopy. Their system may allow AI-enabled fast, miniaturized, and automated LC gas sensors.[107]

LC-based sensors for analyzing gas mixtures containing ozone (O_3) and chlorine (Cl_2) have been showcased by Bao et al.[108] They employed CNNs to process spatiotemporal optical data to identify O_3 and Cl_2 and quantify their concentrations. Their sensor employed LCs supported on metal perchlorate-decorated surfaces where gases diffuse through LC films and undergo redox reactions. 3-D CNNs processed the LC film's spatial and temporal responses to the targeted gases to allow quantitative gas sensing and provide insights into the sensor response to physical processes. The CNNs could extract feature information encoded in the spatiotemporal color patterns of the LCs to detect and quantify the target gases in mixtures by recognizing O_3 from the brightness transition time of the LC and Cl_2 based on late-developing color fluctuations. The method developed by Bao et al. is generalizable to various analytes, reactive surfaces, and LCs, suggesting the potential for portable LC monitoring solutions for gas mixture analysis.[108]

Implementation of AI in Emerging Gas Sensor Technologies. Ultrasonic sensing is a noninvasive technique that can monitor impurity gas composition when combined with neural networks. Zhuang et al. employed a CNN to predict the ultrasonic response and time-of-flight-based ultrasonic signals following excitation to determine the concentrations of argon and air in mixtures with helium. The CNN showed high accuracy in detection and concentration predictions.[185] In other novel sensor technological developments, Yaqoob et al. investigated thermal-conductivity-based MEMS resonators combined with the SVM algorithm to detect He, Ar, and CO_2. Their demonstration achieved a classification accuracy of 100% in a compact and efficient gas sensing platform.[186]

Lithium-ion batteries are widely used for their high energy density and long cycle life. However, safety concerns arise from

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gas leakage during thermal runaway, leading to potential fire and explosion risks. Thus, developing gas monitoring integrated within battery safety management systems is crucial. Current MOS gas sensors generally operate at temperatures higher than the typical working range of lithium-ion batteries, making integration challenging. Hence, there is a need for novel room-temperature gas-sensitive materials. A strategy using ML-based sensor systems to monitor lithium-ion batteries for safety has been proposed by Hu et al.[36] Hu et al. developed sensors based on the perovskite $CsPbBr_3$, functionalized with copper acetylacetonate, which have room-temperature sensitivity to gases of interest in battery thermal runaway, including HF, CO_2, CO, H_2, CH_4, C_2H_4, benzene, ethers, aldehydes, and alcohols. They used ML integration to interpret sensor signals to provide gas detection with efficiency and sufficient time resolution for battery monitoring.[36]

Surface acoustic wave (SAW) technology coupled with ML has demonstrated significant potential in gas sensing.[187−189] The performance of SAW devices is critically influenced by their design and relies heavily on accurate modeling, and thus traditional approaches face challenges due to dependence on precise material properties. ML techniques have been reported to refine coupling of mode theory parameter extraction,[189] enhance the robustness of sensing mechanisms,[187] and decouple multiparameter interferences in thin-film SAW devices via SVM and RF[188] potentially to improve toxic gas (ammonia, nitrogen dioxide, hydrogen sulfide, and other gases) detection.[187] A γ-Fe_2O_3 nanoparticle-coated QCM sensor was recently reported to demonstrate high sensitivity and reliability in detecting SO_2 gas at trace concentrations at room temperature, with an artificial neural network model effectively correlating sensor responses to its concentrations.[190]

■ AI−GAS SENSOR INTEGRATION

Integrating AI with gas sensor technologies allows for autonomous, smart, and selective gas sensor systems for real-time applications. Successful AI−sensor integration can lead to the creation of next-generation sensing technologies with enhanced detection limits and improved selectivity. To achieve AI−gas sensor integration, several vital aspects must be addressed, as described below.

Handling Large, Complex, Noisy, Multimodal, and Uncertain Data. The AI method must be capable of managing large volumes of data with complex patterns, noise, and measurement uncertainties. It has been shown that, generally, for a specific learning task, a larger training set yields better performance.[196,197] The volume of data for model training can be augmented for performance gains.[198] The ability to handle multimodal data, such as combining temporal and spatial variations as well as spectra, images, videos, and text across 1-D, 2-D, and 3-D formats simultaneously greatly enhances the predictive capability. It offers solutions to various sensing tasks.[199] Furthermore, multimodal data allows the creation of unified predictive sensing tools that can cluster, classify (gas identity), regress (gas quantity or concentration), and produce representative embeddings or features for custom user-defined tasks.[200,201]

Integrating multiple sensors and modalities offers superior performance compared to single-sensor approaches, enhancing accuracy and robustness.[152] CNNs are particularly adept at finding patterns from image data and can be modified to help learn from time series and volumetric (3-D) data. Combining multiple models can also be beneficial. Pareek and Chaudhury[194] combined two DL-based architectures to identify and quantify gases. The first model, a 1-D CNN ensemble, is a regression model for gas quantification, effectively handling sensor drift and providing accurate concentration measurements. The second model combines a deep belief network with a drift-aware feature adaptation strategy for gas identification, enhancing the robustness against sensor drift. Both models leverage genetic algorithms for automatic hyperparameter tuning, optimizing their performance without requiring extensive manual intervention. This approach not only simplifies the gas identification and quantification process but also improves the accuracy and reliability of the results.[194]

Optimizing Feature Extraction for High-Dimensional Data Sets. While handling complex, noisy, uncertain, and multimodal data is crucial, the number of features used in the model architecture should also be optimized. The choice of features must be tailored to the specific domain. Excluding unnecessary features or dimensions helps to ensure that the AI model is clear. For instance, representing 1-D spectral data as images without any mathematical transformation and using 2-D convolutions can enable learning but may not be the most efficient approach. DL models, particularly CNNs and RNNs, are adept at feature engineering, i.e., generating derived features from raw data, and can be easily combined with other DL models in gas sensing. Extracting information-rich low-dimensional features (embeddings) and combining engineered features from multiple modalities typically result in improved AI−sensor integration. Several studies have highlighted this approach and produced high-performance AI-based gas sensors.[152,171,180] The curse of dimensionality requires carefully implementing feature extraction methods and low-dimensional visualization techniques to integrate AI methods with gas sensors.[202]

Physicochemical Consistency. The input and output data, representations, and model predictions should be physically and chemically sound. Neural networks can take into account governing physics or chemistry in the loss function so that they do not solely rely on data to offer physicochemical consistency.[203−206] Such physicochemical consistency is crucial in ensuring that a model's predictions are physically and chemically meaningful and accurate. This means the data processed by a model must reflect true physical and chemical properties, and its representation should align with established principles. The model's predictions must also be plausible within known physical and chemical laws. The reliability and validity of ML models in scientific and engineering applications greatly rely on this principle.

Trustworthy and Interpretable Models. Ensuring trustworthy and interpretable predictions is crucial to the effectiveness of AI models. Generally, simpler models require fewer explanations and offer more interpretability. Complex models, such as DNNs and large ensemble methods, require specific methods[138,207] to explain their decision-making processes.[208] Interpretable predictions enable users to understand the underlying logic and reasoning of the model, making it easier to identify and correct potential biases or errors. Trustworthy and interpretable models build confidence in the model's predictions,[209] ensuring they are physicochemically consistent, accurate, and reliable. This combination of attributes is essential for the successful deployment of ML models and their integration with gas sensors.

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Table 3. Challenges and Potential Solutions for AI-Based Gas Sensors

Area	Challenges	Potential Solutions
Gas Sensor Data	• Acquisition Difficulties: Variabilities due to environmental conditions, sensor drift, and other. Sparse features, noisy data, and irrelevant information.	• Develop data-independent models and use prior learning from previously trained models.
	• Data Quality and Volume: Collecting a large and diverse data set representing all possible scenarios. Poor sampling, insufficient data, and missing important outliers.	• Implement advanced statistical sampling methods to improve data quality.
	• Multi-Modality and Bias: Poorly sampled or biased data and the challenges of integrating multimodal data.	• Utilize data augmentation techniques, including synthetic data generation, transformation, and feature space augmentation.
		• Employ few-shot and long-tail learners.
		• Leverage hybrid sensor arrays to improve accuracy and robustness.
Learning Algorithms	• Feature Learning: Learning relevant local and nonlocal features effectively.	• Utilize advanced AI methods such as generative models, attention models, transformers, and physics-driven models.
	• Outlier Detection: Identify outliers and ensure that models are not overly dependent on initial conditions.	• Explore semisupervised, unsupervised, and self-supervised learning.
	• Spatiotemporal Integration: Integrating spatiotemporal patterns into predictions.	• Implement foundation models, multimodal learning, and reinforcement learning.
		• Use causal feature engineering and transfer learning.
AI−Sensor Integration	• Scalability: Scaling AI models to different data set sizes while maintaining performance.	• Implement multimodal learning and adaptive learning techniques, such as reinforcement learning.
	• Sensor Drift and Dynamic Offsets: Sensor drift and dynamic offsets compromise long-term stability, leading to performance inconsistencies.	• Develop real-time drift compensation algorithms and periodic recalibration strategies.
	• Environmental Adaptation: Adapting to rapidly changing or harsh environmental conditions leading to unpredictable sensor behaviors.	• Use sensor fusion techniques, such as Kalman filters or decision-level fusion.
		• Incorporate environmental compensation models to adjust sensor readings based on environmental conditions.
Interpretability and Trustworthiness	• Explainability: Ensuring that AI models and decisions are interpretable.	• Design modular models that allow each component to be inspected individually.
	• Model Complexity: Balancing the complexity of AI models with the need for interpretability.	• Use interpretability techniques, such as SHAP values, LIME, GRAD-CAM, and saliency maps.
	• Transparency: Providing clear explanations for model predictions and identifying potential biases.	• Implement bias mitigation strategies, such as reweighting or adversarial training.
		• Develop user-friendly visualization tools to understand the inner workings of AI models.
Scalability and Environmental Factors	• Resource Constraints: Limited computational resources on sensor devices can restrict the complexity of AI models.	• Implement edge computing strategies.
	• Integration Complexity: Integrating AI models with existing infrastructure and systems.	• Develop lightweight AI models optimized for resource-constrained environments.
	• Environmental Influences: Temperature, humidity, and pressure can affect sensor performance.	• Employ sensor fusion and adaptive filtering techniques.
		• Establish industry-wide standardization protocols and middleware solutions.
Regulatory and Safety	• Compliance and Certification: Adhering to safety and regulatory standards.	• Develop AI-specific standards and certification processes.
	• Lack of Standardization: The absence of standardized guidelines for AI integration.	• Implement model documentation and auditing.
		• Integrate explainable AI techniques.

■ CHALLENGES AND OPPORTUNITIES FOR AI-BASED GAS SENSORS

Integrating AI with gas sensors can advance gas sensor technologies, making systems more autonomous, accurate, and capable of real-time operation. However, several challenges must be addressed to realize these benefits fully. Figure 6 illustrates strengths, weaknesses, opportunities, and threats for AI-based gas sensors, and Table 3 outlines some of the primary challenges and potential solutions for AI−gas sensor integration.

Emerging research suggests that AI can play a transformative role in materials discovery and optimization, accelerating the design of gas-sensitive materials with enhanced properties such as selectivity, sensitivity, and stability.[210] An important consideration for the future of AI-based gas sensors is the integration of AI methods with advancements in materials development. Through ML-driven design of experiments, high-throughput screening, and advanced data analysis, researchers can rapidly explore vast chemical spaces and uncover structure−property relationships that would otherwise remain hidden.[211] AI's predictive ability not only accelerates discovery but also helps refine both experimental protocols and simulation models by closing the loop between theory and practice.[212]

Moving forward, techniques like generative models offer the promise of designing entirely new materials from scratch, guided by target performance metrics.[211,213,214] Meanwhile, explainable AI tools help interpret the "why" behind predictions, fostering trust in results and revealing deeper mechanistic insights.[208,215,216] Ultimately, future research and development will likely feature increasingly autonomous workflows, in which AI, automated synthesis, and real-time characterization collaborate continuously. Embracing this synergy will speed the journey from the initial idea to commercial-ready material. Future research should aim to establish frameworks that tightly couple these disciplines, ensuring that advancements in one domain accelerate progress in the other. This integrative approach may unlock novel

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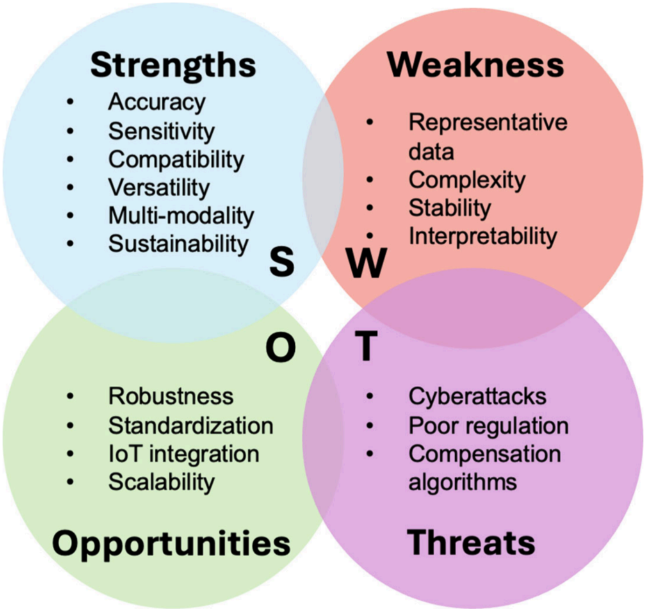

Figure 6. SWOT analysis of the AI-integrated sensors.

pathways for achieving next-generation gas sensors that are not only highly efficient but also adaptive to complex and evolving real-world scenarios.

In summary, integrating AI into gas sensing systems is an area of significant research and development interest, as indicated by the many publications appearing in the last several years. AI can enhance sensor performance, improving gas sensor accuracy, sensitivity, and adaptability. By enabling sophisticated multispecies detection, AI-driven methods pave the way for next-generation sensors that are precise, versatile, autonomous, and adaptable to various applications, from environmental monitoring to industrial process control to medical diagnostics. This review has explored the critical role of AI in advancing gas sensor technologies, the innovative approaches to their integration, and the challenges and opportunities that lie ahead.

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Notes

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LIST OF ACRONYMS

0-D, zero-dimensional; 1-D, one-dimensional; 2-D, two-dimensional; 3-D, three-dimensional; ABDT, adaptive boosted decision tree; AI, artificial intelligence; Bi-LSTM, bidirectional long short-term memory; BLR, boosted linear regression; BRT, boosted regression tree; BAW, bulk acoustic wave; CNT, carbon nanotube; CAE, convolutional autoencoder; CLSTM, convolutional long short-term memory network; CNN, convolutional neural network; DT, decision tree; DBN, deep belief network; DL, deep learning; DNN, deep neural network; DCT, discrete cosine transform; DWT, discrete wavelet transform; EGB, extreme gradient boosting; ET, Extra Tree; GBR, gradient boosting regression; GRU, gated recurrent unit; GPR, Gaussian process regression; GAF, Gramian angular field; ICA, independent component analysis; IR, infrared; k-NN, k-nearest neighbors; kRR, kernel ridge regression; LC, liquid crystal; LDA, linear discriminant analysis; LRC, logistic regression classifier; LSTM, long short-term memory network; MCA, multiple component analysis; ML, machine learning; MOS, metal oxide semiconductor; MEMS, micro-electro-mechanical systems; MLP, multilayer perceptron; MCNA, multiscale CNN with attention; NBC, naive Bayes classifier; NN, neural network; NDIR, nondispersive infrared spectroscopy; PID, photoionization detector; PCA, principal component analysis; PLS, partial least-squares; QDA, quadratic discriminant analysis; QCM, quartz crystal microbalance; RF, random forest; RNN, recurrent neural network; RVM, recurrent vector machine; SLR, simple linear regression; SMCR, self-modeling curve resolution; SVM, support vector machine; SVR, support vector regression; SAW, surface acoustic wave; t-SNE, t-distributed stochastic neighbor embedding; THz, terahertz; TDLAS, tunable diode laser absorption spectroscopy

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