Comparative and Machine Learning-Driven Analysis of Reduced Graphene Oxide–Polymer Gas Sensors: Materials and Sensitivity Trends

Abstract

Gas sensors combining reduced graphene oxide (rGO)–polymer have sparked a growing interest since past few years. rGO–polymers synergistically merge the high surface area and conductivity with the chemical affinity and tunability of polymers, often achieving superior room-temperature gas sensing performance compared to either of the components alone. This review article collates recent advances in rGO–polymer sensors, emphasizing material choices, fabrication techniques, gas detection performance (sensitivity, selectivity, and limits of detection), and specialized applications for nitroaromatic vapor detection. Conducting polymers like polyaniline (PANI), polypyrrole (PPy), polythiophene (PTh), and PEDOT:PSS have been widely incorporated with rGO for the better operation and flexibility for sensing gases like NH_3, NO_2, H_2S, and volatile organic compounds. For these reasons, rGO–polymer sensors represent a rapidly progressing field, with significant steps in tracing toxic industrial gases and explosive compounds. Additionally, this work incorporates a data-driven section where statistical plots and machine learning were used to evaluate performance metrics from published studies. Results show that Limit of Detection (LOD) and gas type are the most influential features affecting sensitivity. Comparative radar charts and heatmaps support a holistic view of material-gas performance, strengthening the future design strategy of rGO–polymer sensors. This interdisciplinary approach supports the transition from experimental sensing platforms to intelligent, application-specific devices for environmental and security applications.

Keywords: reduced graphene oxide, conducting polymer, gas sensor, nitroaromatic compounds, nanocomposite, machine learning.

1. Introduction

Gas sensing is critically important for environmental monitoring, industrial safety, public health, and national security. Detecting toxic industrial gases or explosive vapors at low concentrations can save lives. Traditional gas sensors often require high operating temperatures or suffer from poor selectivity. In this context, Reduced GO - polymer based gas sensors have emerged as attractive alternatives in recent past [1]. These hybrid materials leverage the synergy between rGO and polymers: rGO provides a high surface-to-volume ratio and excellent electrical conductivity, making it highly sensitive to adsorption of gas molecules [2], while polymer contribute specific chemical interactions and flexibility. The result is often enhanced gas sensing performance at room temperature, including higher sensitivity and faster response. Numerous studies have explored rGO–polymers for detecting a wide range of gases – from toxic industrial gases (e.g., NH_3, H_2S, NO_2, CO) to volatile organic compounds and even traces of explosive nitroaromatic vapors (e.g., nitrobenzene, TNT, DNT) [3]. In this review, author has summarized the recent advancements in rGO–polymer-based gas sensors. In the following sections, we examine performance trends for each major gas category, linking differences in sensitivity to the underlying working mechanisms and citing recent experimental findings to support these discussions.

This review also integrates a machine learning (ML) based analytical framework to derive quantitative insights from published experimental data [4]. Using statistical visualization and Random Forest regression, authors have examined the various influencing parameters—such as polymer type, gas type, operating temperature, and LOD on the sensitivity of sensors. The ML-driven feature importance analysis and comparative plots offer a data-backed perception on material–gas performance. This dual approach, combining literature with computational evaluation, aims to support rational design strategies for next-generation rGO–polymer-based gas sensors.

2. Materials and Fabrication Techniques

2.1 Polymer Choices: Conducting polymers have been the most widely used component in rGO-polymer sensors due to their intrinsic conductivity and gas-reactive doping behaviour [3]. Common examples include polyaniline (PANI), polypyrrole (PPy), polythiophene (PTh), and poly(3,4-ethylenedioxythiophene) (PEDOT, typically used as the PEDOT:PSS formulation when blended with poly (styrene sulfonate)). By undergoing charge transfer or doping/de-doping reactions upon binding of gas molecules, these polymers translate gas adsorption into electrical resistance or current changes. In the rGO–polymer composite, the polymer provides selective binding or chemical affinity for certain gases, while rGO serves as a high-surface-area conductive network that facilitates electron transport. For instance, poly(ethylene glycol) (PEG), which is non-conducting, has been used to assemble rGO into supramolecular networks, enhancing adsorption of analyte molecules and thereby improving sensitivity [5]. In some cases, researchers employ molecularly imprinted polymers (MIPs) – functional polymer matrices polymerized in the presence of a target analyte to create selective binding cavities that match the target's molecular shape [6]. Such imprinting endows the composite with highly selective binding sites for those analytes.

2.2 Composite Synthesis Methods: A variety of fabrication techniques have been reported for integrating rGO with polymers into sensing films:

- **In-Situ Chemical Polymerization:** This is a common method where the monomer (e.g., aniline for PANI or pyrrole for PPy) is polymerized oxidatively (or thermally) in the presence of dispersed graphene oxide (GO) sheets, which are simultaneously reduced to rGO during the process. Singh et al., used in-situ oxidative polymerization of aniline in the presence of GO and montmorillonite clay, yielding a PANI/MMT–rGO nanocomposite for hydrogen cyanide (HCN) gas detection [5]. Such in-situ approaches ensure good interfacial contact and charge transfer between the polymer and rGO components.
- **Electrochemical Polymerization:** In this technique, a thin film of conducting polymer is directly polymerized onto an electrode (which is already modified with an rGO layer) by applying an electrochemical potential in a monomer solution. Zheng et al., adopted this approach to create a PEDOT MIP film on a laser-induced graphene (LIG) electrode for sensing TNT and related nitroaromatics [7]. Electrochemical polymerization allows precise control of the polymer film thickness and uniform coverage on micro-fabricated graphene electrodes.

- **Solution Blending and Casting:** A straight forward fabrication route is to blend rGO into a polymer solution and then cast or drop-coat this mixture onto sensor substrates. For example, PEG–rGO composites have been prepared by dispersing rGO in water with various concentrations of PEG, then drop-casting the mixture into thin films. While solution casting is simple, achieving a homogeneous dispersion of rGO within the polymer matrix can be challenging without surface functionalization or surfactants, as rGO sheets tend to aggregate.
- **Electrospinning:** Electrospinning can produce nanofibrous mats of polymer/rGO composite, which greatly increases the surface area of the sensing layer. Researchers have electrospun a composite of poly(vinylpyrrolidone) doped with pyrene and (3-aminopropyl)triethoxysilane along with rGO, forming PVP/pyrene/APTS–rGO “nanonets” for TNT vapor detection. The inclusion of rGO and aromatic pyrene in the fibers significantly enhanced fluorescence quenching by TNT, enabling sensitive optical detection of that explosive. Recent studies continue to explore electrospun rGO–polymer fibers to leverage their large surface area and porosity for improved gas sensing performance.
- **Other Hybrid Structures:** Beyond binary rGO–polymer systems, there is a growing trend to incorporate nanoparticle additives or form multi-component heterostructures. A recent report describes a cadmium sulfide nanocrystal embedded in a PPy–rGO matrix that functions as a selective H_2S sensor [8]. In another case, Ag nanoparticles decorating a PPy–rGO film on an acoustic wave device significantly boosted the sensor’s NO_2 response [5]. Metallic nanoparticles can catalyze surface reactions or improve charge transport in the composite. Additionally, flexible and printed sensors are emerging: researchers have demonstrated printing rGO–polymer inks on plastic substrates and using laser-scribing to create graphene patterns before polymer coating [9]. These techniques aim to produce wearable or low-cost sensor devices. By incorporating such modifications, rGO–polymer sensors can achieve better usability and more consistent performance.

2.3 Gas Sensing Mechanisms of rGO–Polymer Composites: Gas sensing with rGO–polymer composites primarily rely on changes in electrical resistance due to adsorption/interaction of gas molecules. The mechanisms differ for reducing vs. oxidizing gases:

- **Reducing Gases (e.g., NH_3):** Exposure of a p-type rGO–polymer composite to a reducing gas typically causes electron donation to the material, which can de-dope a conducting polymer or supply electrons to rGO, thereby increasing the resistance. In case of ammonia (NH_3) detection using an rGO–PANI composite, PANI is in its conductive emeraldine salt form with delocalized polycation and charge-compensating anions [10]. Upon exposure to NH_3, the ammonia molecules are adsorbed and deprotonate the PANI, converting it to the insulating leucoemeraldine base form by removing protons. This interrupts the conjugation and drastically increases the resistance of the composite sensor. Overall, the NH_3 molecules reduce charge carriers in PANI, leading to a measurable resistance rise [10]. This mechanism shows that PANI-based composites have strong responses to ammonia, with sensitivity enhanced by rGO’s and effective charge percolation network.
- **Oxidizing Gases (e.g., NO_2):** For p-type composites, an oxidizing gas like NO_2 will withdraw/accept electrons, effectively doping the material further which decreases the resistance, enabling detection of trace NO_2 levels

through this charge-transfer mechanism. The high affinity of NO_2 for electron-rich sites and the combined effect between rGO and polymer components allow these sensors to achieve ppb-level detection of NO_2 [11]. In addition to resistance change, it is worth noting that some rGO–polymer composites can exhibit optical responses (e.g., fluorescence quenching) when detecting specific analytes, particularly in the case of nitroaromatic compounds. The underlying sensing principles, however, generally revolve around electron donor–acceptor interactions and modulation of charge carriers in the composite.

3. Performance Trends and Detection Limits

Recent studies show that rGO–polymer sensors have achieved notable improvements in sensitivity, selectivity, and low detection limits across a range of target gases even at room temperature.

3.1 Ammonia (NH_3)

rGO–polymer composites with amine-rich polymers are particularly responsive to ammonia (NH_3). Fabio Seiti Hadano et al. [12] reported a PANI/rGO nanocomposite thin-film sensor with a sensitivity of ~250% (resistance change) at 100 ppm NH_3. In their device, rGO was distributed as nano-clusters within the PANI matrix, providing additional adsorption sites and conductive pathways. Similarly, a recent study by Jose Carlos Santos-Ceballos et al. [13] demonstrated flexible sensors composed of Polyaniline-coated laser-induced graphene sensor showing an LOD of 2.38 ppb for NH_3. The large surface area of LIG increases the number of adsorption sites that are available for gas molecules and improves the sensor sensitivity. These results illustrate a general trend: incorporating rGO amplifies the NH_3 response, while the polymer contributes selectivity via specific chemical interactions.

3.2 Nitrogen Dioxide (NO_2)

NO_2 is a strong oxidizing gas that withdraws electrons from n-type materials. Pristine graphene and rGO are known to be NO_2-sensitive; however, polymer–rGO composites can dramatically enhance sensitivity and allow reliable operation in ambient air. More recently, Shuo Xiong et al. [14] demonstrated a 3D porous architecture of Ag-decorated rGO-polyoyrrole hybrid aerogels. This rGO-PPy/Ag-based Surface Acoustic Wave (SAW) sensor with the UV activation exhibits a high sensitivity 127.68 Hz/ppm, fast response time (36.7s/58.5s), excellent reproducibility and selectivity and fast recoverability. Notably, the addition of Ag nanoparticles and the 3D porous composite architecture improved both sensitivity and response/recovery speed in this device. In another study, a flexible sensor using ethylenediamine-functionalized rGO/PTh film showed roughly 4× higher NO_2 response than pure PTh, consistent with the earlier observation that chemical modification of rGO and composite formation greatly boosts PTh's sensing performance [15]. Overall, rGO–polymer composites tend to exhibit decent selectivity for NO_2 against reducing gases.

3.3 Hydrogen Sulfide (H_2S)

Conducting polymer composites also show strong responses to H_2S, a toxic reducing gas. Many polymers (especially PANI and its derivatives) react with H_2S, and rGO in the composite provides a conductive backbone that enables room-temperature H_2S sensing. A study by Ragab et al. [8] developed a CdS-PPy/rGO chemoresistor that was highly selective to H_2S in air with remarkable response of 98.98% to 70 ppm of H2S gas. In another approach, S.A. Al-Balawi et.al. [16] demonstrated POT/GO sensor with threefold improvement when compared to pure POT, with a maximum response of 99% at 100ppm H2S with a rapid response of 90 s and recovery of 85s times. An advantage of polymer/rGO sensors for H_2S is that they generally operate at ambient temperature, unlike traditional metal-oxide H_2S sensors that often require elevated operating temperatures (≥150 °C) to function. This low-power, room-temperature operation is a significant benefit for wearable or portable H_2S monitors.

3.4 Volatile Organic Compounds (VOCs) and Others

rGO–polymer composites have been investigated for detecting various VOCs such as alcohols, aromatic solvents, and other organic vapors. For example, PEDOT:PSS is a polymer that can respond to polar organic vapors by swelling or changing conductivity. Manoj Kumar et al. [17] demonstrated highest sensitivity, with a 52% response at 200 ppm methanol. This sensor demonstrated good selectivity, long-term stability and reproducibility. Further, Ferry Chrismiadi Nalle et al. [18] demonstrated application of PMMA–rGO Nanocomposite in a Quartz Crystal Microbalance (QCM) sensor for Alcohol-Series VOC Detection with significant improvement in performance. In general, rGO composites achieve respectable sensitivity and improved stability for VOCs under varying humidity, making them attractive for real-world indoor air quality monitoring.

4. Applications for Nitroaromatics

Nitroaromatic compounds (e.g., nitrobenzene and the nitrotoluene isomers 2,4-DNT and 2,4,6-TNT) are associated with explosives and toxic pollutants. Nitroaromatic vapors present a particularly challenging target because of their very low vapor pressures (particularly TNT) and the need for extremely low detection limits. Detection of these compounds is a critical application of advanced gas sensors in security and environmental monitoring. rGO–polymer composites offer new approaches to tackle this problem by combining π–π interactions (from graphene's aromatic surface), specific chemical binding sites from polymers, and signal amplification mechanisms. Several notable strategies have emerged:

- **Molecularly Imprinted Polymer Sensors:** Zheng et al. [7] developed an imprinted PEDOT polymer on a LIG electrode that can concurrently detect a suite of nitro-explosives with outstanding selectivity. This sensor could specifically detect TNT, 2,4-DNT, 1,3,5-trinitrobenzene (TNB), picric acid (TNP), and related compounds each at low-ppb concentrations in a single device.
- **Chemiresistive and Acoustic Wave Sensors:** Graphene and rGO can bind nitroaromatic molecules via π-stacking and charge-transfer, and this effect can be enhanced by functionalizing graphene with polymers or aromatic receptor molecules. Early works demonstrated that fluorescent polymers with appended pyrene groups on rGO could achieve ~80–90% fluorescence quenching by TNT/DNT vapors [19].
- **Fluorescent Nanocomposites:** Besides electrical sensing, optical methods using rGO composites have also advanced. A recent study introduced a luminescent sensor for nitrobenzene gas based on a composite of nitrogen-doped graphene quantum dots (N-GQDs) embedded in a porous metal–organic framework [20]. Nitrobenzene molecules adsorb into the porous matrix and quench the photoluminescence of the embedded N-GQDs. In

principle, a similar strategy could involve fluorescent conjugated polymers blended with rGO, where explosive binding causes a measurable fluorescence decrease. Such optical sensors can reach very low LODs, but typically require specialized optical instrumentation to detect fluorescence changes.

In summary, rGO–polymer composites are proving exceptionally useful for nitroaromatic sensing. Continued innovations in this area are moving laboratory demonstrations closer to practical explosive detectors that could be used by security personnel or for environmental surveillance of remediation sites.

5. Challenges

Despite the promising performance of rGO–polymer sensors, several challenges remain before these composites can see widespread commercial or field deployment:

- **Humidity and Environmental Interference:** Many polymer-based sensors are sensitive to humidity. Polymers can absorb water vapor from the air, which can alter the sensor's baseline resistance or temporarily occupy active binding sites, thereby reducing sensitivity to target gases. For example, a hygroscopic polymer like PANI or PEDOT:PSS may swell or change conductivity in high humidity **[9]**. Ideally, future designs will incorporate features to make the sensors "humidity-insensitive" [10].
- **Stability and Repeatability:** Ensuring long-term stability of rGO–polymer sensors is crucial. Polymers can undergo aging, oxidation over time, leading to drift in sensor response. rGO can gradually re-oxidize or aggregate. This may require stabilizing additives or device self-calibration routines.
- **Selectivity and Cross-Sensitivity:** While polymer functionalization and imprinting have improved selectivity, cross-sensitivity to other gases or vapors can still occur. One approach is to incorporate on-chip filters or scrubbers that remove interferents. Another is to use sensor arrays with pattern recognition algorithms: an array of rGO–polymer sensors, each optimized for different interactions, can collectively distinguish analytes via a 'fingerprint' response pattern. Data-driven techniques (machine learning) are increasingly being applied to classify gases based on responses from multiple sensors, modifying the limitation of any single sensor's specificity.
- **Integration and Power:** To deploy rGO–polymer sensors in real-world applications, integration with low-power electronics and wireless communication is needed. Noise reduction and signal amplification techniques might be required for detecting very low concentrations. Flexible or wearable formats require that sensors be integrated on lightweight substrates and possibly powered by small batteries or energy harvesters.

In summary, while rGO–polymer composites have demonstrated excellent gas sensing capabilities in research settings, efforts to overcome environmental susceptibility, to ensure stability and reproducibility, and to incorporate the sensors into complete devices will determine how soon these technologies can be adopted in practice. The current outlook is optimistic, given rapid progress on multiple fronts including materials stabilization, smart sensor calibration, and flexible device engineering.

6. Future Directions

Research since 2020 indicates several exciting future directions that are likely to shape the next generation of rGO–polymer gas sensors:

- **Advanced Functionalization and Selective Materials:** Future sensors will employ tailored functional groups and novel polymers to improve selectivity. Like, molecular imprinting can create polymer layers that selectively bind a specific target, incorporation of biomimetic receptors or covalently grafted chemical receptors on rGO surfaces, designing polymers that respond only to a certain analyte through specific chemical interactions, doping rGO with heteroatoms (N, S, B, etc.) can change its affinity for certain gases and forming composites of rGO with other 2D materials could create hybrid sensing layers with unique selectivity profiles. Computational chemistry and machine learning may assist in synthesising new conducting material optimized for particular gas targets [10].
- **Improved Nanostructuring for Sensitivity:** A larger surface area generally means more binding sites and a stronger sensor response per analyte concentration. Techniques like electrospinning, 3D printing, or templating porous films all serve to increase the accessible surface area for gas adsorption. One recent concept demonstrated a 3D-printed graphene aerogel decorated with quantum dots to detect formaldehyde at the ppb level – a strategy that could be extended to rGO–polymer systems **[10]**. Nano structuring not only boosts sensitivity but can also improve response speed by allowing gases to diffuse rapidly through the porous network.
- **Multi-Modal Sensing and Sensor Arrays:** Combining multiple sensing mechanisms in one device, or deploying arrays of diverse sensors, will likely enhance reliability and analyte discrimination. Guo et.al have worked on dual-mode SAW + resistive sensor for TNT that provided both frequency and resistance changes [11]. Meanwhile, electronic nose (e-nose) systems using an array of rGO–polymer sensors are under development. In such an array, each sensor is made with a different polymer (or functionalization), and the collective response pattern serves as a fingerprint for specific gases or mixtures [10].
- **Flexible, Wearable, and IoT-Integrated Sensors:** Thanks to the intrinsic flexibility of polymers and the ease of printing graphene-based inks, a major direction is the development of flexible and wearable gas sensors. Researchers have already demonstrated, for instance, PANI–rGO sensors printed on flexible substrates like PET film or textiles, creating wearable badges for ammonia monitoring **[17]**. PEDOT:PSS-based composites have been inkjet-printed or spray-coated to make thin, conformable sensors on plastic foils [9]. The vision is that such sensors could be integrated into clothing or personal protective equipment, continuously monitoring the wearer's environment for hazardous gases and transmitting data wirelessly to smartphones or IoT networks.

In summary, rGO–polymer gas sensors are a rapidly evolving technology. Progress in materials design, composite fabrication, and device integration has led to sensors with lower detection limits, better selectivity, and improved stability. Continued interdisciplinary research – spanning materials science, nanotechnology, and data science – is driving these sensors toward real-world applications such as environmental monitoring, industrial safety, healthcare, and security. With ongoing innovations, it is conceivable that inexpensive, wearable sensor patches or smartphone-linked detectors based on rGO–polymer composites will become reality in the near future.

7. Data-Driven Insights and Comparative Evaluation

To enhance this review with a quantitative layer, Machine Learning approach has been used to analysis with extracted data from recent rGO-polymer gas sensor studies published between 2020 and 2025. This approach aimed to identify key factors which are responsible for sensor performance, explore material–gas relationships, and provide visual insights for better material selection [21]. The dataset used in the analysis was manually compiled from journal articles published between 2020 and recent past, focusing on reduced graphene oxide (rGO)–polymer composite gas sensors. Performance metrics including sensitivity, LOD, response time, target gas, and type of polymer were extracted from experimental studies.

- **Methodology**: Machine learning regression analysis using Random Forest model was implemented using scikit-learn to predict sensitivity (%) as the target variable. The input features included: Polymer type, Gas type, rGO wt%, Operating temperature, and LOD. This model has revealed that LOD was the most predictive feature for sensor sensitivity, contributing over 50% to the model’s output variance. This is followed by the nature of the target gas and the polymer matrix, highlighting the critical role of material–gas interactions. This analysis in Figure 1 highlights that LOD and gas–material interaction play the dominant roles in sensor sensitivity, guiding future experimental focus.

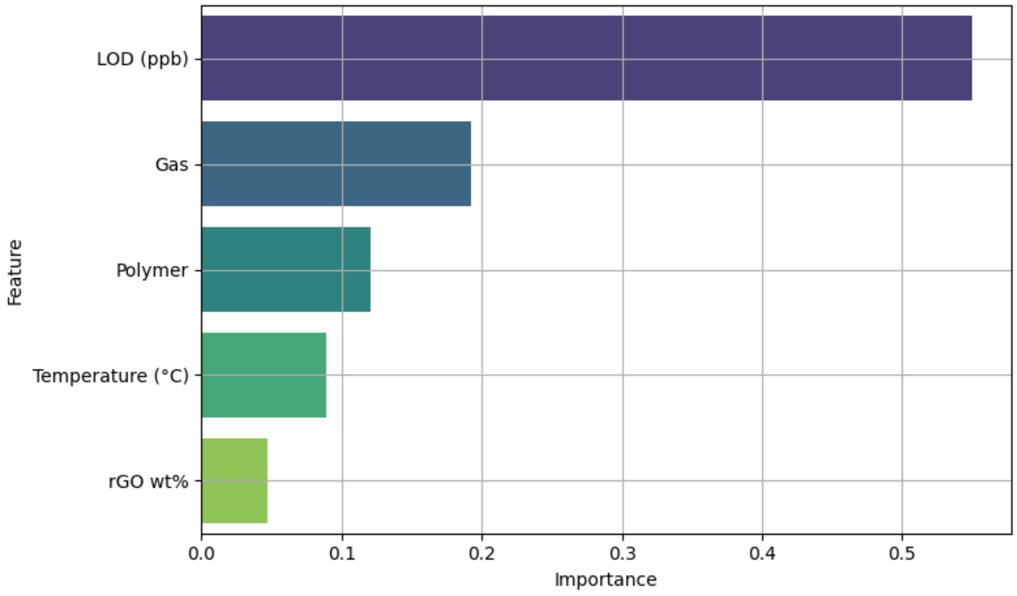

Figure 1

- **Heatmap Visualization:** Two heatmaps were generated based on sensitivity (%) vs. Polymer–Gas combinations and response time (s) vs. Polymer–Gas combinations. Figure 2 shows a heatmap of average sensitivity values of various rGO–polymer composites toward different gases. Polypyrrole (PPy) exhibited the highest sensitivity toward NO_2 (~320%), followed closely by PTh and POT for H_2S detection. PEDOT also demonstrated strong performance for NH_3. In contrast, PANI-based sensors showed moderate sensitivity across the tested analytes. These results support the strategic pairing of polymers with specific gases to maximize performance. Figure 3 presents a heatmap of average sensor response time (s) for rGO–polymer composites toward different gases. PEDOT/NH_3 and PPy/NO_2 exhibited the fastest responses at 45 s and 40 s, respectively. In contrast, PANI-based sensors showed notably slower responses, particularly for TNT detection (180 s). These findings underscore the importance of polymer selection not only for sensitivity but also for rapid detection, which is critical in real-time monitoring scenarios.

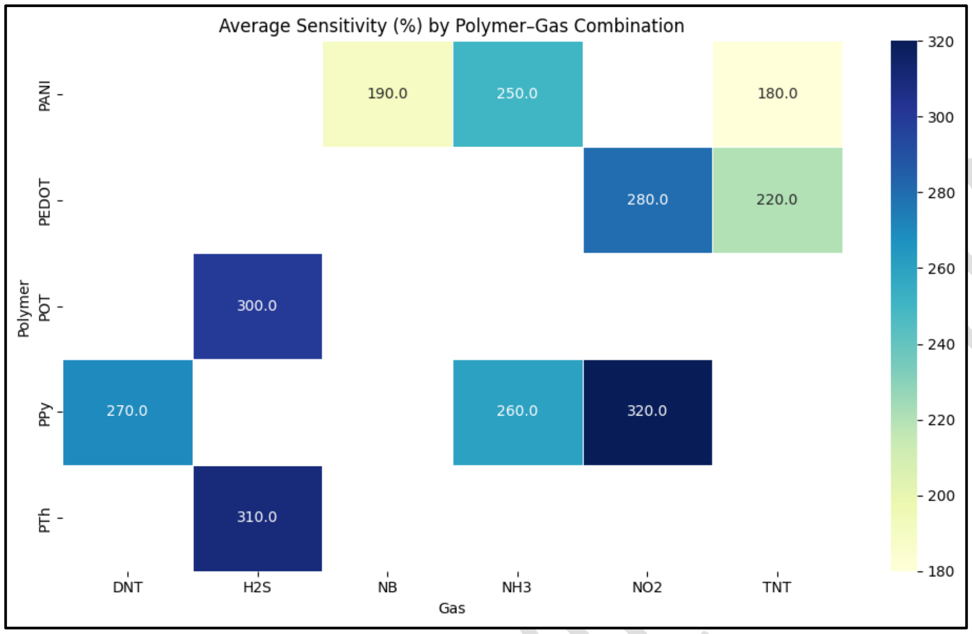

Figure 2

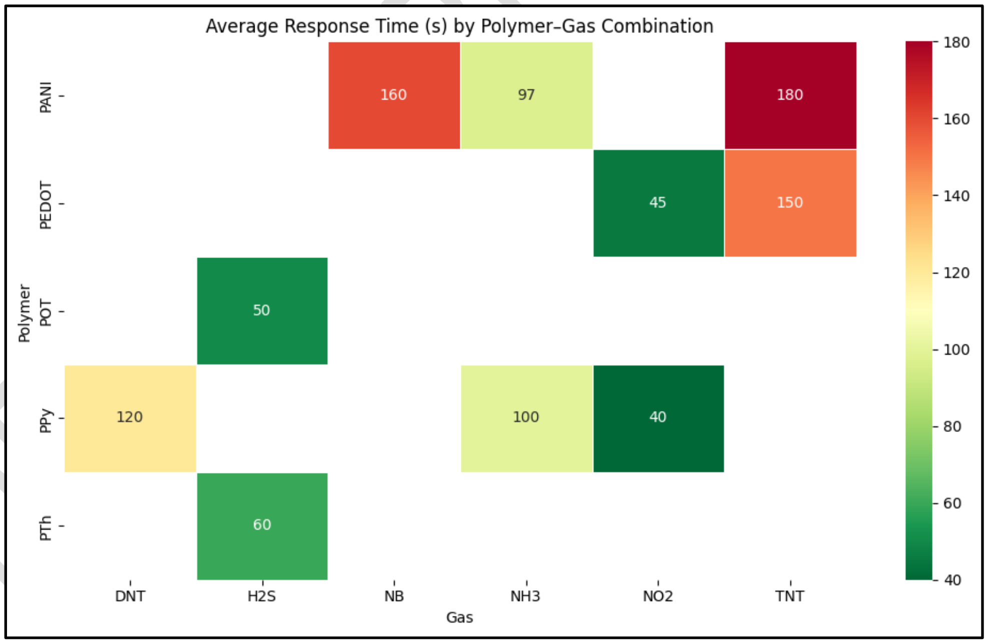

Figure 3

- **Radar Chart Comparison:** To provide a overall comparison of performance, a radar chart was developed to evaluate four representative polymers (PANI, PEDOT, PPy, and PTh) based on normalized metrics, including sensitivity (%), inverse limit of detection (LOD), and inverse response time. It can be observed from the Figure 4 that PTh exhibited the highest sensitivity overall, followed closely by PPy, which maintained strong and balanced performance across all metrics. PEDOT-based sensors demonstrated excellent detection limits but had slightly slower response times. In contrast, PANI-based sensors showed relatively weaker performance, particularly in LOD and response speed. These insights support the strategic selection of polymer matrices for specific gas sensing applications, balancing sensitivity with practical responsiveness.

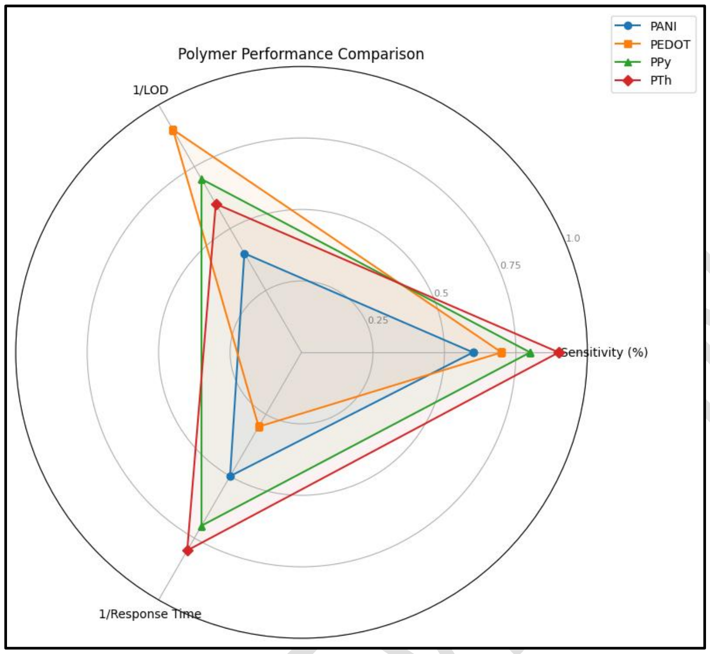

Figure 4

8. Conclusions

In conclusion, **rGO–polymer composites** have emerged as a highly promising platform for gas sensing with the unique integration of two material classes: the high surface area, conductivity, π-electron network of rGO, and the rich chemistry and processability of polymers. Researchers have improved sensor **sensitivity** while maintaining low power consumption by choosing appropriate polymer components and fabrication techniques. Through materials engineering and novel device designs, challenges such as environmental stability, humidity interference, and device-to-device variability are actively being addressed. Practical implementations with prototypes of flexible wearable gas sensors and multi-sensor arrays connected to machine learning for analyte discrimination is under progress. Given the rapid pace of advancement, rGO–polymer composite sensors are expected to play a significant role in the next generation of gas sensing technologies for real-world monitoring of environmental pollutants, industrial gases, and security threats. The machine learning-based insights, when combined with experimental observations, offer a promising data-driven foundation for guiding the rational design of rGO–polymer gas sensors. The approach not only validates known trends but also uncovers new avenues for material pairing and optimization.

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Figure Captions:

Figure 1: Feature importance in predicting sensitivity in %

Figure 2: Average sensitivity (%) vs. Polymer–Gas combinations

Figure 3: Average response time by polymer-gas combination

Figure 4: Performance comparison chart