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From Atoms to Applications: A Comprehensive Review of Graphene Materials and Metal Ion Doped Gas Sensor

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Abstract: Graphene, a two-dimensional allotrope of carbon composed of sp^2 -hybridized atoms arranged in a hexagonal lattice, has emerged as a transformative material bridging fundamental physics and advanced engineering applications. This review presents a comprehensive analysis of graphene, covering its atomic structure, electronic properties, synthesis techniques, and characterization methods, with a particular emphasis on its application in gas sensing. This study further integrates the metal-ion functionalization, specifically rubidium-modified graphene, for the enhancement of sensing performance. Metal doping alters the graphene's electronic structure that improves charge transfer mechanisms, and increases adsorption energy, thereby significantly enhancing sensitivity and selectivity toward gases such as liquefied petroleum gas (LPG) and hydrogen (H_2). Experimental findings demonstrate that 1.0 M Rb-modified graphene achieves superior sensitivity factors (~ 225 for LPG and ~ 241 for H_2 at 390 K).

Keywords: Graphene, Rubidium modified Graphene, Sensitivity, LPG Sensor, Hydrogen Sensor.

I. INTRODUCTION

The discovery of graphene in 2004 revolutionized condensed matter physics and nanotechnology. As a single atomic layer of carbon atoms arranged in a honeycomb lattice, graphene exhibits extraordinary electrical, mechanical, and thermal properties. These arise from its reduced dimensionality and unique electronic band structure characterized by Dirac cones. Despite its exceptional properties, pristine graphene exhibits limited gas sensing performance due to weak adsorption and low selectivity. This limitation has driven research toward metal-ion doping, where foreign atoms modify the electronic structure and enhance gas interaction.

This review integrates:

- Fundamental physics of graphene
- Synthesis and characterization techniques
- Metal-ion modification strategies
- Gas sensing studies

II. LITERATURE REVIEW

Graphene research has undergone a remarkable evolution since its isolation in 2004, transitioning from fundamental scientific exploration to advanced technological applications.

In the initial phase (2004–2010) of graphene research was primarily focused on understanding its fundamental physical properties. Early investigations established graphene as a prototypical two-dimensional material exhibiting exceptionally high carrier mobility and unconventional quantum Hall effects, arising from its linear energy-momentum dispersion near the Dirac points. Mechanical characterization further revealed extraordinary properties, including an intrinsic tensile strength of approximately 130 GPa and a Young's modulus approaching 1 TPa. These findings not only confirmed graphene's superior mechanical robustness but also highlighted its potential for applications in nanoelectronics and structural materials, thereby laying the scientific foundation for subsequent research advancements.

In the second phase (2010–2020) emphasized the development of scalable synthesis techniques and strategies for tailoring graphene's intrinsic properties. Techniques such as chemical vapour deposition, mechanical exfoliation, and chemical reduction of graphene oxide enabled controlled production of graphene with varying quality and defect densities. During this period, functionalization emerged as a critical approach to enhance graphene's applicability. Methods including chemical doping, defect engineering, and the formation of hybrid nanostructures were extensively investigated to modify their electronic, optical, and surface properties. These advancements were particularly significant for applications in sensing, catalysis, and energy storage, where surface interactions and electronic tunability play a crucial role.



Furthermore, Balram et al. (2024) demonstrated that graphene–metal sulfide hybrid nanocomposites exhibit significantly enhanced sensitivity, selectivity, and environmental stability due to synergistic interfacial interactions. Recum and Hirsch (2024) provided a comprehensive analysis of graphene as a chemoreceptive sensing material, emphasizing that metal and heteroatom doping can effectively modulate its electronic structure and adsorption characteristics, thereby improving sensing performance. Francis et al. (2024) highlighted the advantages of laser-induced graphene sensors, particularly their scalable fabrication, high porosity, and large active surface area, which are beneficial for environmental monitoring. Furthermore, Aviraj Teli et al. (2024) reviewed recent functionalization strategies that enhance adsorption kinetics and electronic response. At the device level, Owais et al. (2025) reported successful integration of graphene into MEMS-based gas sensors, achieving rapid response, low power consumption, and enhanced operational reliability. Lu et al. (2025) demonstrated the development of flexible graphene-based composite sensors exhibiting high sensitivity and mechanical adaptability, while Qu et al. (2025) presented a comprehensive review of metal–graphene hybrid systems focusing on performance optimization and sensing mechanisms. Gautam et al. (2025) reported improved LPG sensing using two-dimensional materials, and Liyanage et al. (2025) emphasized the effectiveness of metal-assisted strategies for hydrogen sensing applications.

In the recent era, focus has mostly been on integrating graphene into practical devices, especially in the domains of gas sensing, flexible electronics, and microelectromechanical systems. The high surface-to-volume ratio and exceptional electrical conductivity of graphene make it highly sensitive to environmental perturbations, positioning it as a promising material for gas sensing applications.

Despite these advances, metal-ion modified graphene, particularly involving alkali metals such as rubidium, remains insufficiently explored. Most existing studies predominantly focus on transition metal or metal oxide functionalization, leaving a significant gap in understanding the influence of alkali metal doping on graphene’s electronic structure, adsorption behaviour, and sensing performance.

Therefore, the present study investigates rubidium-modified graphene as an advanced sensing material to enhance sensitivity, selectivity, and sensor efficiency.

III. BACKGROUND OF QUANTUM CONFINEMENT AND MODIFICATION IN GRAPHENE

Graphene’s two-dimensional structure provides high electron mobility and a large surface area, making it highly sensitive to changes in surface charge upon gas adsorption. Metal atom functionalization introduces localized electronic states that enhance charge transfer, modifying the density of states near the Fermi level.

While pristine graphene is a zero-bandgap material, rubidium incorporation introduces localized states that increase gas adsorption energy and amplify resistance changes, resembling quantum confinement effects seen in nanoscale structures. This improves sensor response by altering charge distribution and electronic pathways on the graphene surface.

Graphene exists in several forms [3-5], depending on its structure are shown in Table 1.1

Graphene	Key Features	Common Applications
SLG	Single layer, highest mobility	Electronics, sensors
FLG	2–5 layers	Flexible devices, composites
GO	Oxygenated, insulating	Bio-applications, membranes
Rgo	Partially reduced	Conductive films, energy storage
GNR	Narrow ribbons	Nanoelectronics
GQD	Quantum dots	Bioimaging, LEDs
3D Graphene	Porous 3D structure	Batteries, supercapacitors
Doped	N, B, S, P added	Sensors, catalysis

TABLE 1.1 TYPES OF GRAPHENE, ITS FEATURES AND ITS APPLICATION AREAS

IV. STRUCTURE AND FUNDAMENTAL PHYSICS OF GRAPHENE

A. Atomic Structure:

Graphene consists of carbon atoms arranged in a two-dimensional hexagonal lattice, where each atom is bonded to three neighbouring atoms via strong sp^2 covalent bonds. The remaining p-orbital electrons form delocalized π -bonds, which are responsible for contributing to high conductivity.

B. Electronic Band Structure:

One of the most remarkable features of graphene is its linear energy-momentum relationship near the Dirac points. Charge carriers in graphene behave as massless Dirac fermions, resulting in high carrier mobility and unusual quantum Hall effects. The electronic properties of graphene arise from its unique band structure, which can be derived using the tight-binding approximation. The energy dispersion relation for graphene is as,

$$E(\mathbf{k}) = \pm t \sqrt{1 + 4 \cos\left(\frac{\sqrt{3}k_y a}{2}\right) \cos\left(\frac{k_x a}{2}\right) + 4 \cos^2\left(\frac{k_x a}{2}\right)} \tag{1}$$

Where, t is the nearest-neighbour hopping parameter (~ 2.7 eV), a is the lattice constant, k is the wave vector.

Near the Dirac points, the dispersion relation simplifies and becomes linear

$$E(k) \approx \hbar v_F \|k\| \tag{2}$$

where $v_F \approx 10^6$ m/s is the Fermi velocity.

This linear dispersion indicates that charge carriers behave as massless relativistic particles, and their dynamics can be described by a two-dimensional Dirac-like equation

$$H = v_F \sigma \cdot p \tag{3}$$

Where, H is the Hamiltonian operator, v_F is the Fermi velocity, σ is the Pauli matrices, and $p = -i\hbar \nabla$ is the momentum operator.

This formulation explains several unique properties of graphene: Zero bandgap behaviour, High carrier mobility, Anomalous quantum Hall effect and Klein tunnelling phenomena.

C. Mechanical and Elastic Properties:

Strong carbon-carbon bonding gives graphene extraordinary stiffness and tensile strength.

V. EXPERIMENTAL METHODOLOGY

A. Synthesis and Characterization Techniques:

Graphene can be synthesized by various methods, viz. Mechanical exfoliation, Chemical vapour deposition (CVD), Reduction of graphene oxide, and liquid-phase exfoliation. But the present work employs chemical route techniques due to simplicity, cost-effectiveness, and scalability.

Graphene materials are characterized by various techniques, viz. Raman spectroscopy for defect analysis and layer identification, X-ray diffraction for structural evaluation, Scanning and transmission electron microscopy for morphology, and electrical and thermal measurements for transport properties. These techniques establish direct correlations between structure and performance.

B. Materials:

Commercial graphene powder with high purity was used as the base material for synthesis. Rubidium salt of analytical grade was employed as the dopant source without purification. All chemicals were procured from standard suppliers and used as received. Deionised water was used throughout the synthesis process.

C. Synthesis of Rubidium-Modified Graphene:

Rubidium-modified graphene was synthesized by the chemical route technique. A known quantity of graphene powder was dispersed in rubidium-containing aqueous solutions with varying molar concentrations. The mixtures were continuously stirred to ensure homogeneous dispersion and effective interaction between graphene and rubidium.



Fig 1: Stepwise Synthesis of Rb Modified Graphene

The resulting suspensions were chemically processed to facilitate uniform incorporation of rubidium within the graphene matrix. After completion of the reaction, the samples were dried at a controlled temperature to remove residual solvents. The dried powders were subsequently annealed to improve structural stability and dopant integration. The obtained Rb-modified graphene powders were used for characterization and sensor fabrication.

D. Characterization

1) XRD Characterization:

X-ray diffraction confirmed the graphene structure and indicated successful rubidium incorporation. Scanning electron microscopy revealed that Rb addition increased surface roughness and dispersion, which enhances the adsorption of gas molecules. The XRD patterns of pure graphene and Rb-modified graphene show a characteristic peak at approximately 26.6°. The peak positions for all samples are consistent, indicating reproducible structural features. Analysis of the patterns reveals information about the crystallinity and phase of the materials. While the pristine graphene exhibits a predominantly amorphous nature, the incorporation of rubidium leads to enhanced crystallinity, as evidenced by sharper and more defined peaks in the Rb-doped samples.

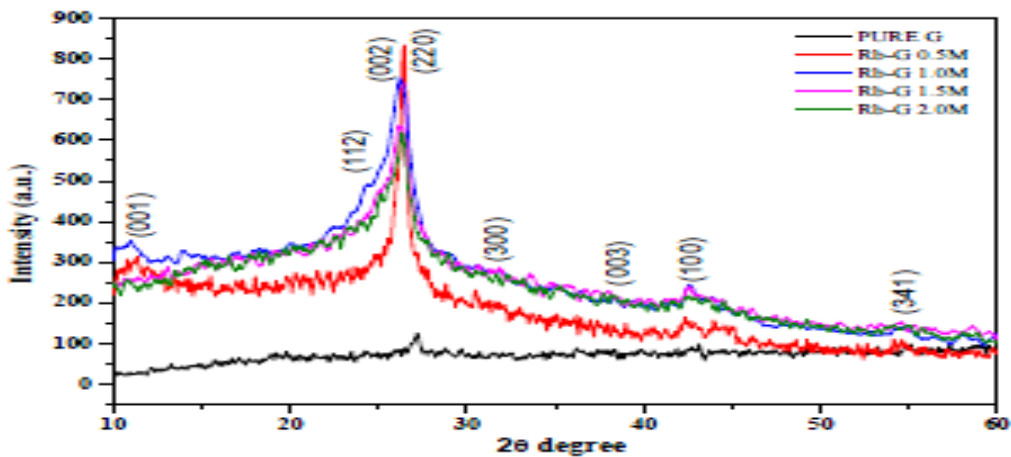


Fig. 2 XRD of Graphene and Rb-Modified Graphene Nanoparticles

2) SEM Characterization:

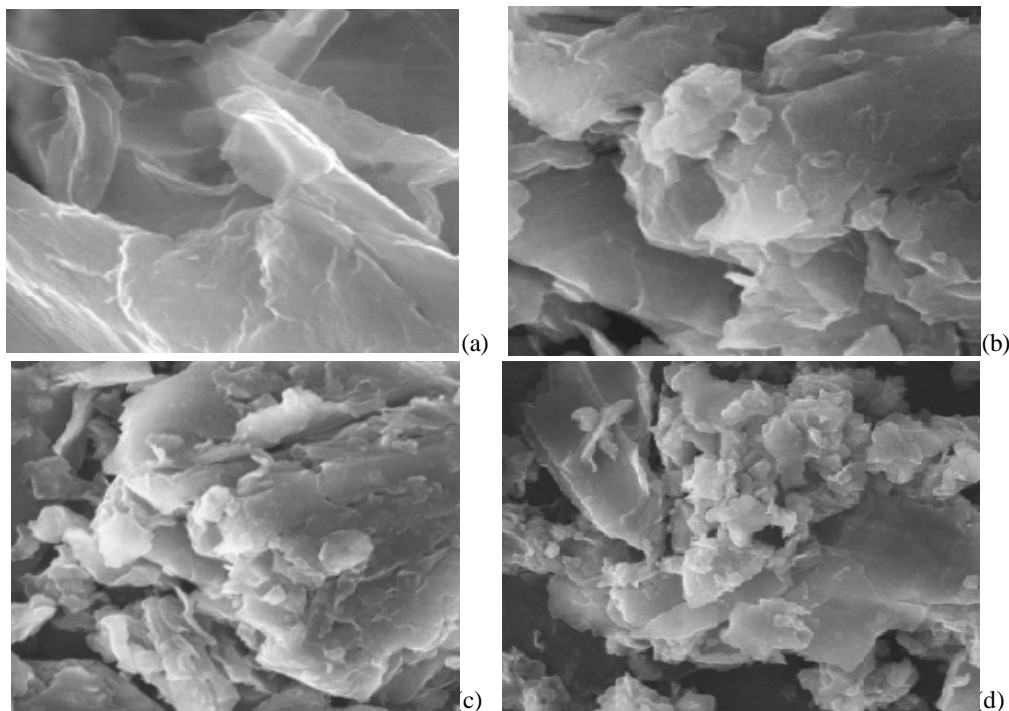


Fig. 3. SEM Images of (0.5,1.0,1.5,2.0 M) Rb Modified Graphene Nanoparticles SEM images of 0.5 M, 1.0 M, 1.5 M and 2.0 M concentrations of Rb-modified graphene are presented in Figure 3 (a,b,c,d). The morphology of nanostructures is strongly influenced by Rb in graphene. The pristine graphene has a smooth surface with tightly packed sheets, whereas the exfoliated graphene appears as transparent, wrinkled layers, indicating extensive exfoliation and well-formed sheet structures that represent Rb concentration, which induced the changes in surface morphology, reflecting the effect of dopant levels.

Characterization	Observation	Effect of Rb Incorporation
XRD	Peak at 26.6°	Confirms graphene, slightly shift due to Rb
SEM	Layered and wrinkled structure	Increased surface roughness and dispersion with Rb

TABLE 1.2. SUMMARY OF STRUCTURAL AND MORPHOLOGICAL CHARACTERISTICS

E. Sensor Fabrication

Powders were pelletized and silver electrodes applied for conductivity measurements.

F. Gas Sensing Measurements (Electrical Characterization)

Sensors were exposed to LPG and hydrogen in the range 380–390 K. Sensitivity factor was calculated as:

$$SF = \frac{R_a - R_g}{R_g}$$

where Ra is the resistance of the sensor in air, and Rg is the resistance in presence of targeted gas.

Sensor performance was evaluated by measuring resistance changes upon exposure to LPG and H₂ at temperatures between 380 K -390 K. The sensitivity factor (SF) quantified the response: 1.0 MRb-modified graphene showed SF ≈ 225 for LPG at 390 K, SF ≈ 241 for H₂ at 390 K. i.e., 1.0 M Rb-modified graphene exhibits the highest sensitivity for both LPG and H₂.

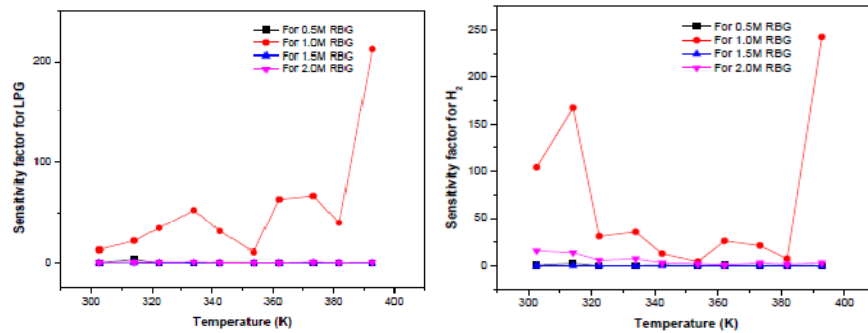


FIG 4: SENSING RESPONSE OF (0.5,1.0,1.5, 2.0 M) Rb MODIFIED GRAPHENE (A) LPG, (B) H₂

Rb Concentration (M)	Gas	Operating Temperature (K)	Sensitivity Factor (SF)
0.5	LPG	390	13
1.0	LPG	390	225
1.5	LPG	390	16
2.0	LPG	390	15

TABLE 1.3 RUBIDIUM MOLAR CONCENTRATION VS LPG GAS SENSITIVITY

Rb Concentration (M)	Gas	Operating Temperature (K)	Sensitivity Factor (SF)
0.5	H ₂	390	13
1.0	H ₂	390	241
1.5	H ₂	390	19
2.0	H ₂	390	17

TABLE 1.4 RB MOLAR CONCENTRATION VS H₂ GAS SENSITIVITY

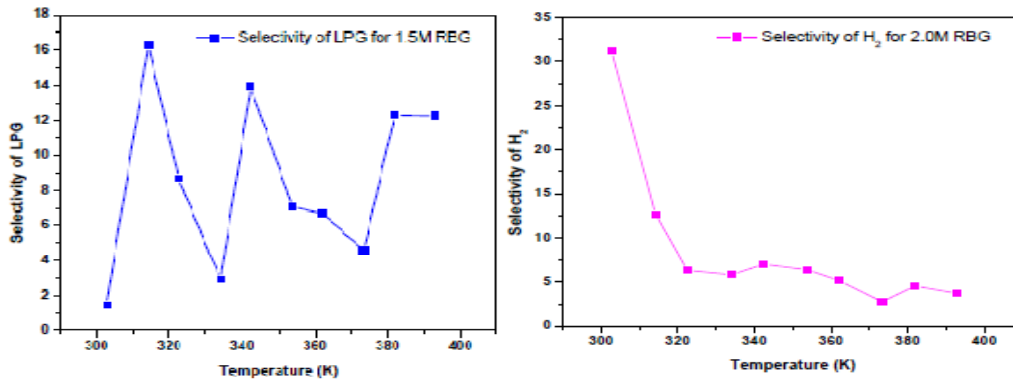


FIG.5 SELECTIVITY OF RB (1.5, 2.0 M) MODIFIED GRAPHENE (A) LPG, (B) H₂

Selectivity analysis showed improved discrimination between LPG and hydrogen gases with increasing Rb content.

VI. RESULTS AND COMPARATIVE ANALYSIS

Gas sensitivity shows a maximum response at 1.0 M Rb concentration, with SF values of 225 (LPG) and 241 (H₂), indicating optimal performance compared to other concentrations. Structural analysis (XRD) confirms a graphene peak at ~26.6°, validating the material’s formation. SEM reveals a layered, wrinkled morphology due to Rb incorporation, enhancing surface area and gas adsorption.

A. Gas Sensitivity:

Rb Concentration (M)	LPG: Sensitivity Factor (SF)	H ₂ : Sensitivity Factor (SF)
0.5	13	13
1.0	225	241
1.5	16	19
2.0	15	17

TABLE 1.5 GAS SENSITIVITY

B. Structural and Morphological Changes:

Property	Observation	Effect of Rb Incorporation
XRD	Peak at 26.6°	Confirms graphene
SEM	Layered and wrinkled structure	Better adsorption

TABLE 1.6 STRUCTURAL AND MORPHOLOGICAL CHANGES

VII. DISCUSSION

The enhanced sensing performance of Rb-modified graphene can be explained by Rubidium atoms providing active adsorption sites, increased surface roughness that improves gas interaction and electron transfer, which alters the resistance significantly of Rb doped sample. That means doping transforms graphene from a passive conductor into an active sensing material.

VIII. APPLICATIONS

Gas sensing technologies have wide applications in safety, industry, and smart systems. They are used for LPG leakage detection and hydrogen sensing to prevent accidents in domestic and industrial environments. In industrial safety, these sensors help in transformer fault detection and the monitoring of hazardous gases. With advancements in technology, they are integrated into IoT-based networks for real-time environmental monitoring and smart system applications.



IX. CHALLENGES AND FUTURE SCOPE

The development of sensing materials faces challenges such as large-scale production, stability of doped materials, and reproducibility of results. These limitations affect their consistency, reliability, and commercialization potential. Future advancements are expected through hybrid nanocomposites, AI-integrated smart sensors, and flexible wearable sensing devices for improved performance and real-time applications.

X. CONCLUSION

This review establishes a direct connection between atomic-level physics and real-world engineering applications of graphene. While pristine graphene offers exceptional intrinsic properties, metal-ion doping significantly enhances its functional performance, particularly in gas sensing applications. Rubidium-modified graphene demonstrates remarkable sensitivity and selectivity, making it a promising candidate for next-generation sensing technologies. Future advancements in synthesis, doping strategies, and device integration will further unlock graphene's potential in sustainable smart systems.

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