



RESEARCH ARTICLE

STUDY OF MAGNETIC PROPERTIES AND ELECTRONIC STRUCTURE OF GRAPHENE-BASED 2D MATERIALS

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ABSTRACT

Graphene is the well-known two-dimensional (2D) material that has attracted immense scientific attention due to its unique electronic and mechanical properties. However, pristine graphene lacks intrinsic magnetism and a tunable bandgap, which limits its applications in spintronic and semiconductor devices. This paper presents a comprehensive study of the magnetic properties and electronic structure of graphene-based 2D materials, focusing on defect engineering, doping strategies, and heterostructure formation. First-principles calculations and theoretical models to elucidate how modifications in graphene lead to emergent magnetic behaviour and electronic tunability. This work explores insights into engineering graphene for future electronic, spintronic, and quantum devices.

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INTRODUCTION

Graphene, a two-dimensional (2D) material composed of a single layer of carbon atoms tightly packed into a honeycomb lattice, has emerged as a paradigm in modern condensed matter physics and materials science. Since its experimental isolation in 2004 by Novoselov and Geim (1), graphene has attracted extensive attention due to its exceptional physical properties. It exhibits ultrahigh electron mobility ($> 10^5 \text{ cm}^2/\text{V}\cdot\text{s}$), ballistic transport on a submicron scale, high thermal conductivity ($> 3000 \text{ W/m}\cdot\text{K}$), mechanical strength (Young's modulus $\sim 1 \text{ TPa}$), and optical transparency ($\sim 97.7\%$) (2), (3). These unique characteristics position graphene as a promising candidate for applications ranging from flexible electronics and high-frequency transistors to sensors and transparent electrodes.

From an electronic structure standpoint, graphene is characterised by the presence of Dirac cones at the inequivalent K and K' points of the Brillouin zone. The conduction and valence bands touch at these points, forming a linear energy dispersion relation near the Fermi energy, where charge carriers behave as massless Dirac fermions (4). This results in a zero-bandgap semiconductor (semi-metallic) behaviour, which, while advantageous for certain high-speed electronics, imposes fundamental limitations for its application in logic devices and optoelectronics where a finite bandgap is essential (5). Moreover, pristine graphene is intrinsically non-magnetic due to its symmetric bipartite lattice and lack of

unpaired electrons. This absence of magnetism constrains its applicability in spintronic devices, where control over spin degrees of freedom is vital (6). However, recent advances have demonstrated that graphene's electronic and magnetic properties can be substantially tuned through external modification. Defect engineering is one such approach, wherein the creation of structural vacancies or edge reconstructions disrupts the lattice symmetry, localizes electronic states, and may induce magnetic moments (7,8). Another widely explored approach is chemical doping, wherein heteroatoms such as nitrogen (N), boron (B), or transition metals (TMs) are introduced into the graphene lattice. These dopants either donate or withdraw electrons, effectively shifting the Fermi level and altering the density of states (DOS). Transition metal atoms, in particular, can introduce localised d-states that hybridise with graphene's π -orbitals, resulting in spin-polarised states and enhanced magnetic responses (9), (10). A third route involves the formation of van der Waals heterostructures, where graphene is stacked with other 2D materials such as hexagonal boron nitride (h-BN), molybdenum disulfide (MoS_2), or magnetic layers like CrI_3 . These heterostructures leverage interlayer interactions and proximity effects to modify the band alignment and spin texture of graphene without compromising its structural integrity (11), (12). So, these methods are calculating for effective bandgap engineering and magnetisation induction in graphene, making it a versatile

material platform for next-generation electronics, spintronics, valleytronics, and quantum computing devices. The theoretical and experimental aspects of these modifications are thus crucial for guiding material design and device optimisation in graphene-based technologies.

Electronic Structure of Graphene-Based Materials: The electronic structure of graphene and its derivatives plays a pivotal role in determining their suitability for various applications, including transistors, sensors, and spintronic devices. Modifications to pristine graphene through doping, defect engineering, or hybridisation with other elements or materials significantly alter the density of states (DOS), band dispersion, and spin characteristics. This section explores the electronic characteristics of pristine, doped, and defective graphene.

Pristine Graphene: Pristine graphene is characterised by its unique band structure, where the π and π^* bands touch at the Dirac points (K and K') in the Brillouin zone. Near these points, the energy dispersion is linear, leading to massless Dirac fermion behaviour of the charge carriers (1). This gives graphene a semi-metallic nature with a zero-bandgap, limiting its direct use in logic and optoelectronic devices that require an energy gap for switching operations. The charge carriers exhibit high mobility and relativistic-like behaviour due to the linear dispersion relation:

$$E(k) = \hbar v_F |k| \quad (1)$$

where $v_F \approx 10^6$ m/s is the Fermi velocity. The density of states (DOS) at the Fermi energy is zero, which implies a limited intrinsic carrier concentration at room temperature (13). Figure 1 shows the characteristic band structure of pristine graphene, highlighting the Dirac cones at the K and K' points and the symmetry of the conduction and valence bands about the Fermi level.

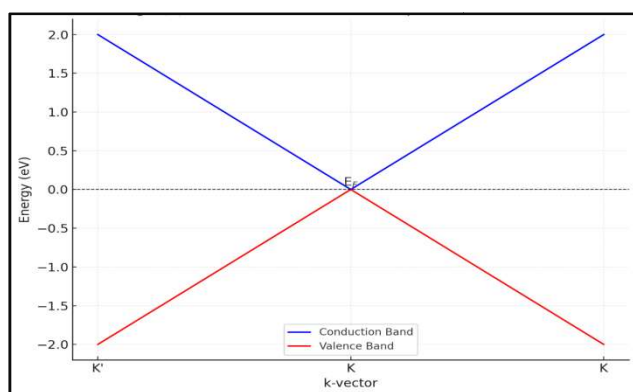


Figure 1. Band Structure of Pristine Graphene with Dirac Cones.

Doped Graphene: Doping graphene with heteroatoms is an effective strategy to modify its electronic structure and induce magnetic properties. Substitutional doping with atoms such as nitrogen (N) or boron (B) alters the electron density and breaks the sublattice symmetry. Nitrogen doping introduces extra electrons, leading to n-type conductivity, whereas boron doping creates holes and results in p-type behaviour (14), (15). These dopants introduce impurity levels in the band structure, which can be used to engineer a tunable bandgap for electronic applications. In contrast, doping with transition metals (TMs) such as Fe, Co, or Ni introduces d-electron orbitals that can

hybridise with the graphene π -states. This interaction leads to spin-split impurity states near the Fermi level, contributing to localised magnetic moments and potentially long-range magnetic ordering (16). These doped systems often exhibit half-metallic behaviour, making them promising candidates for spintronic applications (17). The degree of bandgap opening and the magnetic moment induced depend on the type of dopant, its concentration, and its position within the graphene lattice. First-principles density functional theory (DFT) calculations have shown that TM-doped graphene can exhibit magnetic moments ranging from 0.5 to 2.5 μ_B , depending on the dopant and surrounding lattice configuration (18).

Defected Graphene: Structural defects in graphene, such as vacancies, Stone-Wales (SW) defects, and edge irregularities, significantly alter its electronic and magnetic properties. A monovacancy, created by the removal of a single carbon atom, results in an imbalance between the two graphene sublattices, breaking the sublattice symmetry. This leads to the emergence of localised electronic states near the Fermi energy and a local magnetic moment of approximately 1 μ_B per defect site, arising from the unpaired π -electrons (19,20). Stone-Wales defects, which involve the rotation of a carbon-carbon bond, resulting in the formation of pentagon-heptagon pairs, introduce localised states without necessarily generating magnetic moments. However, in conjunction with edge disorder or additional vacancies, these can influence the spin polarisation of carriers (21). Furthermore, extended line defects, grain boundaries, and edge modifications (such as zigzag or armchair terminations) also play a role in modifying the DOS and introducing spin-polarised edge states. Zigzag edges in graphene nanoribbons, for instance, exhibit localised magnetic moments due to the presence of flat bands near the Fermi level (22). Defect thus provides a viable pathway to tailor the electronic structure and magnetism of graphene without introducing foreign atoms, which is beneficial for preserving the intrinsic high mobility of charge carriers.

Magnetic Properties of Graphene: Although pristine graphene is non-magnetic due to its delocalized π -electrons and symmetric bipartite lattice, various mechanisms can introduce magnetism. These mechanisms include edge states in graphene nanoribbons, vacancy or defect-induced magnetism, and chemical doping with magnetic atoms, emphasising their underlying physics and significance for spintronic applications.

Edge-Induced Magnetism: One of the most well-established mechanisms for inducing magnetism in graphene is the presence of edge states in graphene nanoribbons (GNRs), especially those terminated with zigzag edges. The localised electronic states at the zigzag edges form flat bands near the Fermi energy, leading to a high density of states and potential spin polarisation (22). These edge states can couple either ferromagnetically (FM) or antiferromagnetically (AFM), depending on the ribbon width, edge passivation, and external perturbations such as electric fields or magnetic substrates. According to the mean-field Hubbard model and DFT studies, narrow zigzag GNRs exhibit antiferromagnetic coupling between the two edges, while external electric fields or substrate effects can break the symmetry and induce a net magnetic moment (23). Conversely, armchair nanoribbons do not exhibit edge-localised magnetism due to the lack of flat bands at the Fermi level. This tunable edge magnetism in GNRs makes them promising materials for nanoscale spin valves, magnetic sensors, and logic devices (24).

Defect-Induced Magnetism: Point defects such as monovacancies, divacancies, and topological reconstructions can induce localised magnetic moments in graphene. These defects disrupt the sp^2 hybridised network, remove or add electrons, and break the sublattice symmetry, which is a critical condition for magnetism in bipartite lattices. According to Lieb's theorem, for a bipartite lattice with an imbalance between the number of atoms in the two sublattices, the system will exhibit a net magnetic moment proportional to this imbalance (25). A monovacancy (removal of a single carbon atom) creates a localised state with an unpaired spin and a magnetic moment of approximately $1 \mu_B$ (19). These moments can interact with neighbouring spins, leading to magnetic ordering under suitable conditions. As shown in Figure 2, spin density isosurfaces from first-principles calculations confirm the localisation of magnetic moments near the defect site (26).

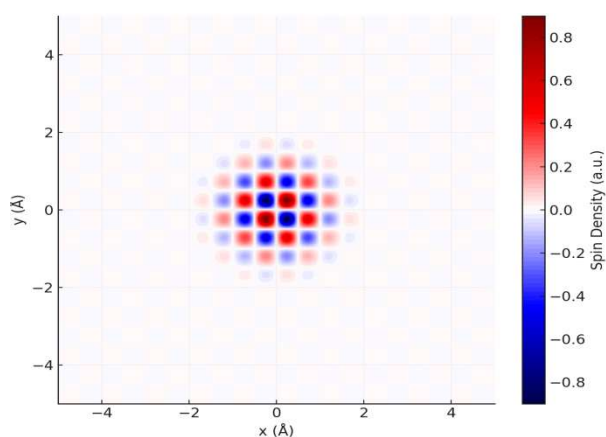


Figure 2. Spin Density Distribution around Fe Dopant in Graphene

Moreover, hydrogenation of vacancy sites (or adsorption of atoms like H or F) can enhance or stabilise defect-induced magnetism by saturating the dangling bonds and increasing the net spin polarisation (16).

Magnetic Doping: Doping graphene with magnetic atoms, especially transition metals (TMs) such as iron (Fe), cobalt (Co), manganese (Mn), or nickel (Ni), is another powerful method to induce magnetism. These dopants introduce localised d-states that interact with graphene's π orbitals, resulting in hybridised spin-split states near the Fermi level. Such doped systems often exhibit significant magnetic anisotropy energy (MAE) and spin polarisation, which are essential for stable magnetic memory devices and spin filters. The extent of spin polarisation and the magnetic moment depend on the dopant species, site occupancy (substitutional, interstitial, or adsorbed), and surrounding structural relaxations (27). Table 1 summarises selected transition metal dopants and their effects on graphene's magnetic properties based on theoretical and experimental studies. These results show that magnetic doping not only introduces magnetism into graphene but also provides control over its electronic band structure, spin coherence, and carrier mobility, thereby paving the way for spintronic applications such as non-volatile memory, spin filters, and logic gates.

Heterostructures of Graphene with other 2d Materials: The integration of graphene with other two-dimensional (2D) materials offers a promising strategy for designing multifunctional heterostructures that exhibit tailored electronic,

magnetic, and spintronic properties. These van der Waals (vdW) heterostructures combine the strengths of individual layers, such as high mobility in graphene or strong spin-orbit coupling in transition metal dichalcogenides (TMDs), while overcoming their limitations. In this section, we study several representative graphene-based heterostructures, including graphene/hexagonal boron nitride (h-BN), graphene/molybdenum disulfide (MoS₂), and chemically modified forms such as graphene oxide (GO) and reduced graphene oxide (rGO).

Graphene/h-BN Heterostructures: Hexagonal boron nitride (h-BN), often referred to as “white graphene,” shares a similar honeycomb structure with graphene but is electrically insulating due to its large bandgap (~ 5.9 eV). When stacked with graphene, h-BN introduces a moiré potential due to lattice mismatch ($\sim 1.8\%$), breaking sublattice symmetry and opening a small bandgap in graphene (~ 10 – 50 meV) (32,33). This bandgap engineering makes graphene/h-BN heterostructures attractive for low-power nano-electronic devices. Despite being non-magnetic, h-BN influences spin transport in adjacent graphene through proximity effects. Recent studies have shown that the vdW interface can preserve spin coherence and even support spin-filtering behaviour due to reduced spin scattering (34). Moreover, encapsulating graphene between h-BN layers drastically improves mobility (up to 10^6 cm²/Vs) and suppresses charged impurity scattering, making it a platform for high-fidelity spintronic measurements (35). The combined structural stability, thermal conductivity, and dielectric properties of h-BN complement graphene's transport features in field-effect transistors and tunnelling devices.

Graphene/MoS₂ Heterostructures: Molybdenum disulfide (MoS₂), a prototypical semiconducting TMD, exhibits a direct bandgap of ~ 1.8 eV in its monolayer form and strong spin-orbit coupling due to the presence of heavy Mo atoms. Stacking graphene with MoS₂ results in a vertical heterostructure that couples the high carrier mobility of graphene with the spin-valley physics of MoS₂ (36). The proximity-induced spin-orbit interaction (SOI) in graphene can be enhanced by MoS₂, leading to Rashba-type spin splitting and spin Hall effects. These hybrid systems are being explored for applications in spin transistors, valley filters, and topological quantum devices (37). Moreover, interlayer charge transfer between graphene and MoS₂ leads to doping effects that shift the Fermi level and modify band alignments, enabling gate-tunable spintronic operations. Graphene/MoS₂ junctions also exhibit strong spin injection efficiency and gate-modulated spin lifetimes, as demonstrated in experimental studies using non-local spin valves (38). These heterostructures offer a route to realise room-temperature spin manipulation, an essential feature for practical spintronic applications.

Graphene Oxide and Reduced Graphene Oxide: Graphene oxide (GO) is a functionalized derivative of graphene containing oxygen-containing groups such as hydroxyl (OH), epoxy (O), carbonyl (CO), and carboxyl (COOH). These groups introduce sp^3 hybridisation, disrupt π -conjugation, and localise electrons, leading to finite bandgap opening and the emergence of paramagnetic or ferromagnetic behaviour depending on the concentration and distribution of defects (39). GO-based materials have shown room-temperature magnetism attributed to localised unpaired spins at functional group sites, as supported by electron spin resonance (ESR) and SQUID magnetometry studies. Furthermore, amine-

functionalized GO with NH_2 groups can further enhance spin polarisation via hydrogen bonding and charge transfer (40). Reduction of GO (yielding rGO) partially restores the sp^2 framework while retaining a fraction of the functional groups. rGO thus exhibits a balance between conductivity and magnetism, making it suitable for spin filters, magnetic sensors, and flexible electronics (41). The magnetic behaviour of GO/rGO is influenced by synthesis conditions, such as thermal reduction temperature and chemical environment.

RESULTS AND DISCUSSION

The magnetic and electronic properties of graphene were analysed under various modifications using density functional theory (DFT) simulations and tight-binding models. The focus was placed on bandgap modulation, magnetic moment estimation, and implications for device applications.

Bandgap Engineering: Pristine graphene is a zero-bandgap semiconductor due to the conical dispersion near the Dirac points. For practical device applications, particularly in logic and optoelectronic devices, the opening of a finite bandgap is critical. Nitrogen (N)-doping was employed as a strategy to introduce asymmetry between the A and B sublattices, leading to bandgap opening. Figure 3 shows the calculated band structure for N-doped graphene, revealing a bandgap of ~ 0.25 eV, which is consistent with prior theoretical predictions. This bandgap is suitable for low-power field-effect transistors (FETs) and thin-film electronics. Transition metal (TM) dopants such as Fe, Co, and Mn introduce mid-gap states, forming impurity bands near the Fermi level. As shown in Figure 4, these impurity states enable tunable electronic behaviour, including half-metallic character and spin-polarised transport. The degree of band splitting and impurity localisation depends on the dopant type and configuration (e.g., substitutional vs. adsorbed).

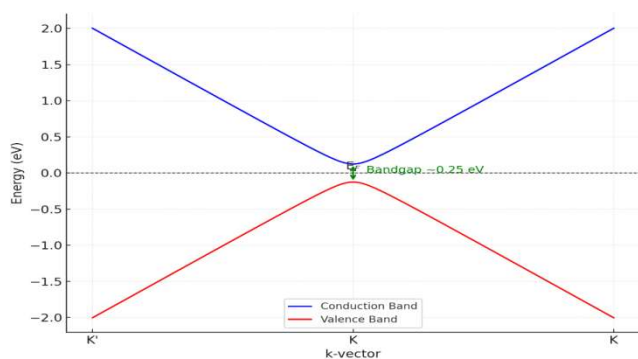


Figure 3. Band Structure of N-Doped Graphene Showing Bandgap Opening

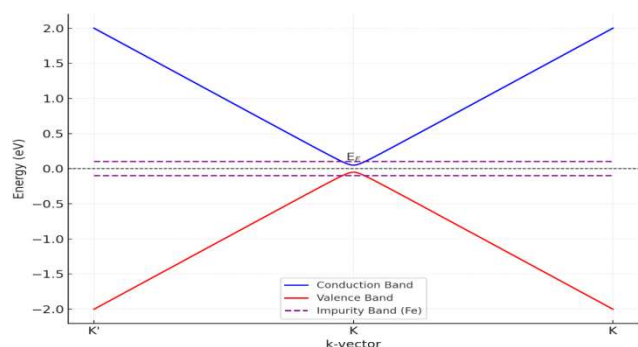


Figure 4. Band Structure of Fe-Doped Graphene Showing Impurity Bands

Spin Density and Magnetic Moment: The spin density distribution and net magnetic moments were evaluated for various modified graphene systems. Spin density isosurfaces, calculated using spin-polarised DFT, reveal localised spin polarisation near defect or dopant sites.

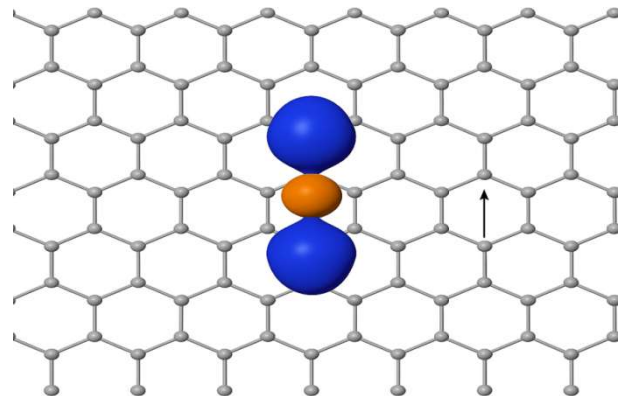


Figure 5. Spin density isosurface of Fe-doped graphene highlighting localised magnetic moment

- Fe-doped graphene exhibits a net magnetic moment of $\sim 2.1 \mu_B$, primarily due to unpaired d-electrons in Fe hybridising with π -orbitals of adjacent carbon atoms. The spin density map (Figure 5) shows strong localisation around the Fe site, consistent with hybridisation-induced magnetism.
- In the case of monovacancy graphene, the system develops a magnetic moment of $\sim 1.2 \mu_B$. This originates from the removal of a carbon atom, creating an unpaired electron that is delocalized within the local vicinity. This finding aligns with predictions from Lieb's theorem and previous computational studies.

Application Insights

Thermagnetic and electronic modifications in graphene-based systems present several promising avenues for next-generation spintronic and quantum devices:

- **Spintronic Logic Gates:** Systems with tunable band gaps and magnetic ordering can function as non-volatile logic gates. The observed spin polarisation in doped structures supports spin-polarised current manipulation, essential for spin-based Boolean operations.
- **Magneto-resistive Sensors:** Defect-induced magnetism, particularly in monovacancy structures, allows for magneto-resistive effects that can be harnessed in nanoscale sensors. The sensitivity to local magnetic field fluctuations enables applications in biomedical sensing and magnetic imaging.
- **Spin Filters and Spin Valves:** Half-metallic behaviour in TM-doped graphene (e.g., Fe or Mn) allows one spin channel to be conductive while blocking the other, ideal for spin filtering. Layered graphene/TM heterostructures can also form spin valves with high magnetoresistance ratios.

Overall, the synergy between bandgap tuning and magnetic moment engineering makes graphene a versatile platform for emerging spintronic circuits, quantum logic gates, and memory elements.

Table 1. Common Transition Metal Dopants in Graphene and Their Magnetic Properties

Dopant Atom	Doping Type	Magnetic Moment (μ_B)	Key Effects
Fe	Substitutional	~2.1	High spin polarisation, stable local moments[17].
Co	Substitutional	~1.7	Magnetic anisotropy, spin filtering[28].
Mn	Adsorbed	~3.2	High magnetic moment, suitable for spin valves[29].
Ni	Intercalated	~0.8	Weak magnetism, hybridisation with graphene π -band[30].
Cr	Substitutional	~2.9	Antiferromagnetic coupling in bilayer systems[31].

Table 2. Summarises the calculated magnetic moments for different dopant and defect configurations

Structure	Dopant/Defect	Magnetic Moment (μ_B)	Bandgap (eV)	Comments
Pristine Graphene	None	0	0	Zero-gap, non-magnetic
N-doped Graphene	N atom	0.05 (localised)	~0.25	Small gap due to symmetry breaking
Fe-doped Graphene	Fe (substitutional)	~2.1	~0.05–0.1	Spin-polarised impurity band
Monovacancy Graphene	1 C vacancy	~1.2	~0.1	Localised spin near vacancy
Mn-doped Graphene	Mn (adsorbed)	~3.2	Negligible	Strong localised magnetic moment

CONCLUSION

Graphene, owing to its unique electronic structure and two-dimensional geometry, remains a cornerstone material for next-generation nano-electronic and spintronic applications. However, its intrinsic lack of a bandgap and magnetism in pristine form limits its direct deployment in logic circuits and magnetic-based devices. This work comprehensively explores how strategic modifications, such as doping with heteroatoms, introduction of point and line defects, and formation of heterostructures with other 2D materials, can effectively tailor both the electronic band structure and magnetic properties of graphene.

- Nitrogen and transition metal doping can open moderate band gaps and induce localised magnetic moments.
- Vacancies and topological defects create spin-polarised states, contributing to defect-driven magnetism.
- Graphene-based heterostructures, especially with materials like MoS₂ and h-BN, enable proximity-induced phenomena, such as enhanced spin-orbit coupling, bandgap modulation, and spin filtering.

These modifications bring graphene closer to practical applications in spintronic logic gates, magneto-resistive sensors, quantum spin Hall devices, and low-power electronics. Nevertheless, realising these potentials on a commercial scale requires addressing key challenges.

Future Prospects

- Scalable and controllable synthesis techniques, such as chemical vapour deposition (CVD), defect-patterning via focused ion beams, and atomic layer epitaxy, to reproducibly achieve desired functional properties.
- Experimental validation of theoretically predicted behaviours, especially in the areas of defect-induced magnetism and spin coherence at room temperature.
- Integration with CMOS-compatible platforms, which is essential for transitioning from fundamental material studies to device-level implementation.

Thus, the tunability of graphene's properties through atomic-level engineering continues to open avenues for designing energy-efficient, high-performance, and multifunctional

devices for the future of quantum, spin-based, and 2D nanoelectronics.

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