EDUCATUM JSMT Vol. 12 Number 2 (2025)
ISSN 2289-7070 / e-ISSN 2462-2451(43-52)
https://ejournal.upsi.edu.my/index.php/EJSMT/index

Density Functional Theory of Graphene and its Hybrid Materials: A Review of Recent Advances and Applications

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Received: 1 July 2025; **Accepted:** 5 October 2025; **Published:** 15 December 2025

To cite this article (APA): Rika N Safitri, et. al., Density Functional Theory of Graphene and its Hybrid Materials: A Review of Recent Advances and Applications. EDUCATUM Journal of Science, Mathematics and Technology, 12(2), 43–52.

To link to this article:

Abstract

Graphene has attracted the attention of researchers as it shows exceptional electrical, mechanical, and thermal properties that are beneficial for various applications, including flexible sensors and supercapacitors. Therefore, much laboratory work was conducted to study further potential application of graphene. However, complex procedures and waste consideration are other challenges for developing graphene-based-application devices. Therefore, using a density functional theory (DFT) to intensively study graphene and its potential to be combined with various materials, resulting in a lower-cost and more efficient approach. This review provides a comprehensive overview of the fundamental theory in DFT, followed by graphene and its hybrids in computational work. Hybridizing graphene with other nanomaterials significantly modifies its bandgap and density of state, which are potential for sensing and electronic devices. Moreover, an in-depth analysis of open-source and commercial software tools used for DFT analysis is also discussed. Despite its advantages, some challenges, including functional accuracy and computational cost, limit the use of DFT analysis. Hence, user-friendly and accessible software is highly required. As a summary, this review serves as a valuable resource for researchers and students, fostering further advancements in graphene-based materials.

Keywords: Graphene; Hybrid Materials; Density Functional Theory; Electronic Structure

INTRODUCTION

Graphene has captivated the scientific community since it was discovered in 2004 due to its extraordinary electrical, mechanical, and thermal properties. It is a promising material for various advanced applications, from flexible electronics to high-performance energy storage devices [1]. Despite its extraordinary properties, restacking due to the van der Waals force and defects might decrease conductivity [2]. Therefore, researchers have been studying the combination of graphene with other materials, such as metal oxides, metals, polymers, and so on, to address these challenges [3], [4], [5], [6].

The research trend from 2020 to 2026 is presented in Figure 1. The data was collected from the Scopus database with the keywords "graphene and its hybrids" and limited to articles and English sources only. For the last five years, there have been 12,635 related documents. As depicted in Figure 1 (a), from 2020 to 2022, there has been a high and stable publication rate, indicating a strong interest among researchers worldwide in graphene and its hybrids. The migration to flexible electronics and the high demand for advanced sensors and energy devices are believed to be the reasons for intensive study on graphene and its hybrids. A slight decline was then observed from 2023 to 2025, as it was predicted due to the shifting focus, rather than synthesis to application-oriented or commercialization studies. Thereafter, this promising graphene will never be underestimated since some publications for 2026 have begun. Furthermore, based on Figure 1 (b), it can be observed that graphene is highly hybridized with inorganic materials such as metals and metal compounds, metal oxides, and semiconductors. Moreover, carbon-based materials such as carbon nanotubes, graphite, graphene oxide, or activated carbon become the second most commonly combined with graphene. Organic materials, including polymers and biomaterials, as well as hybrid structures, can also be hybridized with graphene and offer promising applications.

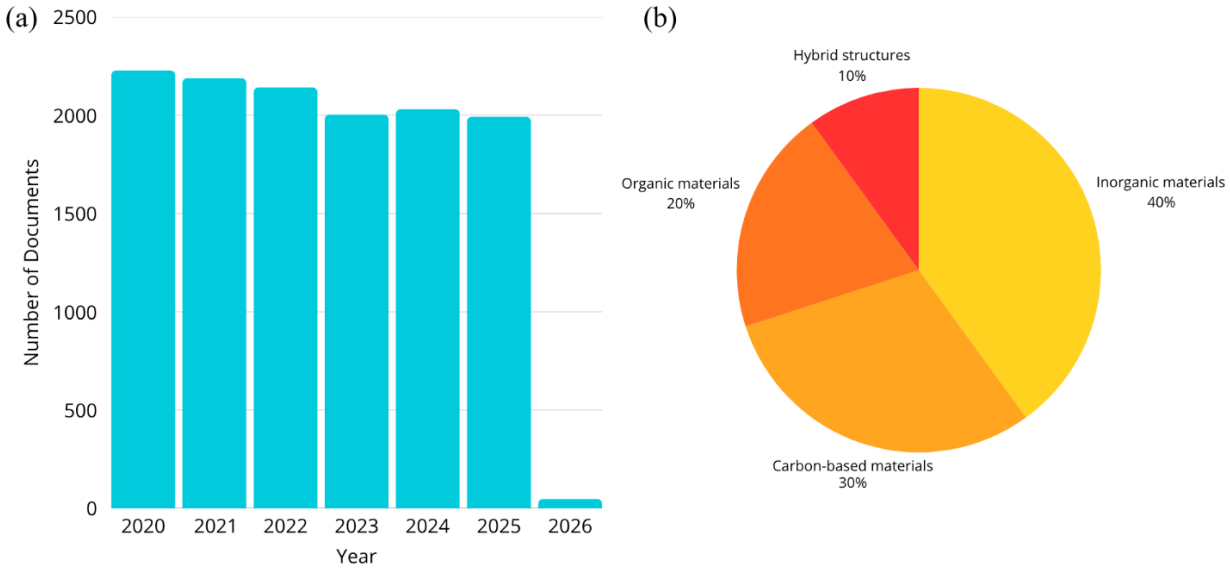

Figure 1. Number of documents published in Scopus on graphene and its hybrids from 2020 to 2026.

The number of publications above indicates the massive studies on graphene and its hybrids [7]. However, it cannot be neglected that the synthesis process might result in waste material. Moreover, the optimization process is time-consuming and absorbs the budget. Therefore, a computational approach is selected to preliminarily evaluate research on graphene, as the optimization process can be conducted in the simulation, which is a waste-free approach, making it more effective and efficient. In this case, a density functional theory (DFT) can be introduced as the initial method to investigate the fundamental understanding of graphene and its hybrid materials [8]. DFT simulations offer some benefits, including being cost-effective and faster to perform than experimental work, allowing for rapid exploration of a wide range of material configurations and conditions. In addition, from DFT simulation, difficult atomic-level

interactions and charge transfer processes can also be studied [9]. Finally, DFT studies can guide the development and optimization of graphene and its hybrid materials in a cost-effective, rapid, and lean manner for further potential applications.

This review aims to offer significant qualitative progress in DFT work on graphene and its nanohybrids in the last few years. This paper covers the theory, electronic structure, and basic applications, and evaluates software tools for DFT. Furthermore, this review highlights the current challenges and limitations of graphene and its hybrid study using a computational approach. The research direction and prospective themes are also discussed to guide experimental physicists and computational scientists in synergistic collaboration in developing innovative and impactful studies on graphene-based systems.

THEORETICAL METHODS IN DFT STUDIES

At the nanoscale, quantum mechanics is crucial for understanding the behavior of nanomaterials as the particle size approaches of the de Broglie wavelength, leading to significant quantum effects such as particle-wave duality. Moreover, the Schrödinger equation is a fundamental equation in quantum mechanics that describes how the quantum state of a physical system changes over time. For a non-relativistic system of N electrons in an external potential $V(\boldsymbol{r})$, the time-independent Schrödinger equation is given as:

$$\hat{\mathrm{H}}\Psi\left(r_{1,}\, r_2, \ldots . r_N\right) = E\ \Psi\left(r_{1,}\, r_2, \ldots . r_N\right) \tag{1}$$

where $\hat{\mathrm{H}}$ is the Hamiltonian operator, $\Psi\left(r_{1,}\, r_2, \ldots . r_N\right)$ is the wavefunction of the system, and E is the total energy of the system. The Hamiltonian of the electron's system typically consists of the kinetic energy, the interaction with external potential (V_{ext}), and the electron-electron interaction [10], as written below:

$$\hat{\mathrm{H}} = -\frac{1}{2}\sum_i^N \nabla_i^2 + V_{ext} + \sum_{i<j}^N \frac{1}{|r_i - r_j|}, \tag{2}$$

where r_i and r_j are the positions of the i-th and j-th electrons, respectively; however, this equation is complicated to solve analytically, and as N increases, the description of a more extensive system becomes prohibitive [11]. Therefore, DFT is developed to simplify the computation of the Schrödinger equation approach. Utilizing the DFT methods, a wide variety of atomic systems, including molecules, surfaces, and electronic devices, can be studied [10]. Hohenberg-Kohn theorems were known as the main principle of DFT [12]. The theorems explain that the ground-state properties of a system can be determined from the electron density alone rather than the many-electron wave function, significantly reducing the computational complexity of the problems. In detail, the Hohenberg-Kohn theorems [12] are stated as below:

Theorem I: "The ground-state electron density $\rho(\boldsymbol{r})$ determines all system properties."
Theorem II: "The ground-state electron density $\rho(\boldsymbol{r})$ is a unique functional of the external potential $V(\boldsymbol{r})$."

Therefore, by developing the Hohenberg-Kohn theorems, the complexity of the Schrödinger equation can be realized as the electron density $\rho(\boldsymbol{r})$ that can be derived from the wavefunction $\Psi(r_1, r_2, \ldots, r_N)$ by integrating the system in one electron coordinate. Furthermore, the ground-state energy can be expressed as a function of the electron density, with the minimum energy achieved by minimizing the energy functional with respect to the electron density. These theorems establish electron density as the fundamental variable in DFT, enabling efficient and accurate calculations for many-electron systems.

Moreover, as the ground-state energy ($\boldsymbol{E_0}$) is obtained by solving the eigenvalue problem for the wavefunction in the Schrödinger equation, the ground-state ($\boldsymbol{E_0}$) in DFT is obtained by minimizing the

energy functional $E[\rho]$ concerning the electron density $\rho(\boldsymbol{r})$. Furthermore, the Kohn-Sham formalism is used to make DFT computationally feasible. The total energy can be computed from the equation below [13]:

$$E_T = \sum_i^M E_i - \frac{1}{2} \int \rho(r)\, V_{(H)}(r) d^3r + \int \rho\,(r) E_{\mathrm{xc}}[\rho\,(r)] - V_{\mathrm{xc}}[\rho] d^3r \qquad (3)$$

The Kohn-Sham equation is solved iteratively to find the electron density [$\rho(\boldsymbol{r})$] that minimizes the functional energy. This process is known as the self-consistent field (SCF) procedure.

In summary, the Schrödinger equation should be solved to obtain a quantum system's complete wavefunction and energy. However, its complexity increases as *N* increases, so analytical solutions are invisible. Hence, DFT offers simplicity in addressing this limitation by focusing on the electron density $\rho(\boldsymbol{r})$, a unique Vext functional. The Kohn-Sham equation in DFT is a single-particle Schrödinger-like equation that approximates the many-body problem through an effective potential. It is agreed that the Schrödinger equation and DFT aim to find the ground-state energy and properties of the system. Still, DFT offers a computationally efficient alternative to solve the complete Schrödinger equation.

OVERVIEW OF GRAPHENE ELECTRONIC STRUCTURE AND PROPERTIES

DFT provides a quantum mechanical model for analyzing the electrical properties of alloys, including two-dimensional alloys, such as graphene. Moreover, DFT is one of the critical analysis tools that helps to study the band structure, density of states (DoS), and carrier dynamics of graphene to explain the semiconducting nature of the material and the high carrier mobility in it.

The electronic band structure of graphene, and especially along the high-symmetry K-point in the Brillouin zone, has a linear relationship between energy and momentum. This linear dispersal results in massless Dirac fermions, which are attributed to the exceptionally high speed of the electron mobility in graphene. Besides, graphene is not subjected to a vanishing DoS at the Fermi level, as is the case with more traditional semiconductors, which is a direct result of its two-dimensional geometry and linear band dispersion [14]. The behaviour of mechanical system in low-dimensional structures is significantly different than that of bulk materials. In 2D material like graphene, the propagation of mechanical stress is governed by a power-law decay proportional to $r^{-(d-1)}$, where *r* is the distance between the point of interest and the point of defect, and *d* is the dimension of the material.

Recent studies based on DFT have focused on the modification of graphene nanostructures with the inclusion of other nanomaterials, including silver nanoparticles (AgNPs) [15], platinum (Pt), palladium (Pd), iridium (Ir), nickel (Ni), copper (Cu) atoms [16], activated carbenes [17], and zinc oxide (ZnO) [18]. These structures are hybrid in character and possess adjustable electronic features, such as tunable band gaps and increased adsorption, which makes them beneficial in sensors, catalysis, and energy applications. For instance, the interaction of graphene and AgNPs has been studied based on DFT analysis using Quantum ESPRESSO software for industrial oil and gas sensors and purifiers [15]. Adding AgNPs shows a strong chemisorption of methane (CH_4). Furthermore, with the addition of other metal nanomaterials, such as Pt, Pd, Ir, Ni, and Cu atoms, the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) gap value of graphene was decreased [16]. Furthermore, the bandgap modification of the graphene/ZnO hybrid was also reported using Quantum ESPRESSO [18]. The calculation of DFT implemented the Quantum ESPRESSO package [19], using a plane-wave basis set and the projector augmented wave method, with the generalized gradient approximation (GGA) developed by Perdew, Burke, and Ernzerhof (PBE) for electron exchange-correlation functional.

Baachaoui et al. reported the DFT investigation of functionalized graphene with activated carbenes for a heavy metal cation sensor. The graphene was prepared in a supercell consisting of 6×6 unit cells with 72 carbon atoms [17]. In their study, the Brillouin zone was sampled using a 3×3×1 Monkhorst-Pack K-

point grid, and the orbital energies were broadened using Gaussian smearing of 0.01 eV. On the other hand, Mohammadi-Manesh and Ahmadvand study the DFT of Ag-doped mono- and bilayer-graphene for gas sensors and purifiers of industrial oils [15]. Using a similar Quantum ESPRESSO package, the monolayer vacancy graphene (MVG) and bilayer vacancy graphene (BVG) were prepared using a 6×6 supercell with a lattice parameter of 14.76 Å. The vacancy was placed in the center of the MVG supercell. In contrast, the BVG was made with a distance of two graphene layers of 3.4 Å and a similar supercell. The DFT calculation was conducted using the PBE exchange-correlation function with the GGA function and van der Waals density functional (vdW-DF) correction. Based on the energy band structure and DoS measurement, Ag impurity changes the energy band structure of MVG and BVG. The absorption of CH_4 gas in the graphene layer with the presence of Ag affects the charge carrier conditions and constraints because of the hybridization of the d orbitals of Ag. It changes the dielectric function, resulting in an electron transport modification. The summary of graphene and its hybrid DFT study is presented in Table 1.

Table 1. The DFT study of graphene and its hybrid material in various applications

Hybrid material	Software	Set parameter	Application	Finding	Ref.
AgNPs	Quantum ESPRESSO	6×6 supercell graphene. The calculation was conducted in the PBE exchange-correlation function using the GGA function and the vdW-DF correction	Gas sensor and purifier of industrial oil	Bilayer graphene/AgNPs show lower bandgap, resulting in good conductivity. However, multi-layer graphene/AgNPs with higher bandgap exhibit higher adsorption potential	[15]
Metal nanomaterials (Pt, Pd, Ir, Ni, Cu)	Gaussian09	Using 6-31 G (d, p) basis set with the wB97XD method	Biosensor lung cancer	Combining graphene and other metal nanomaterials reduced the HUMO_LUMO gap. Among the metal nanomaterials, Cu—and Pt-doped graphene is the best candidate for a biosensor for lung cancer.	[16]
Activated carbenes	Quantum ESPRESSO	PBE correction with supercells of graphene was 6×6	Heavy metal sensor	Based on the simulation, cycloaddition induced a bandgap opening of the graphene. Moreover, varying the pH gives a different sense for cations	[17]
ZnO	Quantum ESPRESSO	Using plane-wave basis set and project-augmented wave method, involved GGA from PBE	-	Combining graphene and ZnO reduces a bandgap of ~ 0.72 eV compared to the experimental bandgap of ~ 3.3 eV	[18]
Silver cluster (Ag_6)	Gaussian09	Using LANL2DZ for effective core potential (ECP) basis set	Gas sensor	the graphene/silver hybrid shows DoS modification near the Fermi level, enhancing sensitivity	[20]

Furthermore, graphene and its hybrid research trend were studied using VOSviewer analysis. The bibliographic data were collected from the Scopus database using the keywords "density functional theory graphene." Moreover, the data was filtered from 2014 to 2025, focusing on only English articles. The network visualization is presented in Figure 2 based on the co-occurrence analysis. Based on the network

visualization figure, the circle represents the items, and the size of the circles indicates a highly discussed topic. Furthermore, the different colors represent different clusters, as the figure can be obtained as six clusters. Each cluster indicates the connection of the items. The red cluster mainly focuses on its electronic structure, including the band gap and first principles. The second cluster, indicated in green, focuses on its analysis procedure; the application in the sensor is represented in blue, while the yellow item indicates catalyst application. As supported in the inserted figure, the research trend is indicated by the items in yellow cycles, which show that catalytic application has become the focus of the study for the last two years.

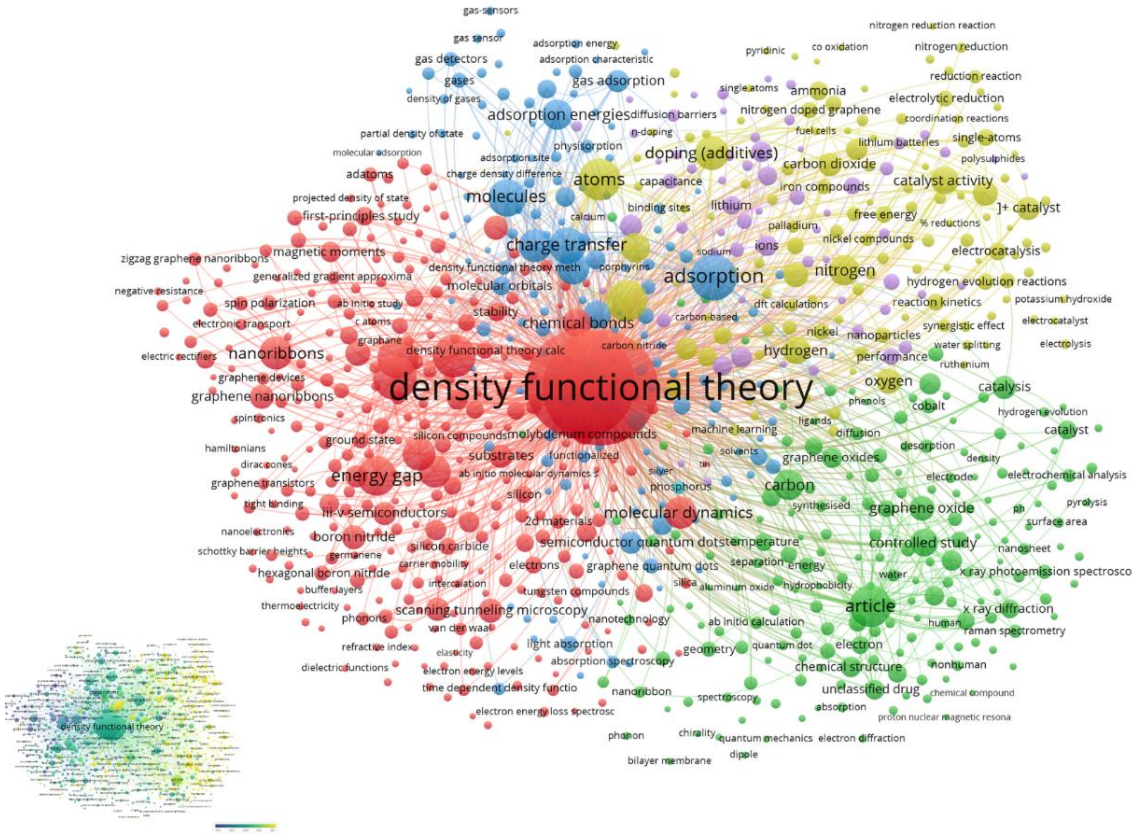

Figure 2. The network visualization of the "density functional theory of graphene" from VOSviewer analysis (data was collected on 31 October 2025)

SOFTWARE TO STUDY DFT OF GRAPHENE AND ITS HYBRID

Computational experiments have become an alternative solution to studying complex systems in science, especially in quantum mechanics. A computer science method can be used to conduct the simulation to analyze and simulate complex systems in this approach. In line with this, a computer experimental study is generally carried out to solve the DFT of graphene, including open and commercial software. The crucial components in any DFT simulation during the computational analysis are Pseudopotentials, exchange-correlation functionals, K-point sampling, spin polarization, and modules [21]. To perform reliable DFT simulations, these components or key parameters should be carefully considered.

Pseudopotentials are crucial in DFT calculations for graphene and other materials. This software can reduce computational complexity, enhance accuracy and reliability, improve convergence and stability, be flexible and easy to customize, and ensure consistency with experimental data. The simplification in this technique can be obtained by eliminating the need to explicitly treat core electrons, making the simulation

possible in large or complex systems, since only the valence electrons are being simulated. Therefore, this Pseudopotential setting allows user to model larger supercell even for a complex graphene/hybrid system.

Understanding the exchange-correlation functional is the next important feature in DFT calculations. At the atomic scale, the electrons are repelling each other rather than being closer. Theoretically, from a quantum mechanics perspective, the repulsion is not only a common Coulomb force but also involves the exchange effect from the Pauli exclusion principle. Therefore, in the DFT analysis, this complex interaction is simplified and represented as an exchange-correlation functional. Typically, the exchange-correlation functional consists of Local Density Approximation (LDA), GGA, meta-GGA, hybrids, and meta-hybrids [21]. The LDA describes that the exchange-correlation functional is simplified by considering the location's spin density. To extend, GGA includes density derivatives. Furthermore, the meta-GGA is known to be a more accurate approximation that combines density and gradient. The next exchange-correlation functional offers better accuracy, yet complexity.

Furthermore, the K point data analysis is essential for electronic structure information, as it provides information on the Brillouin zone, band structure, and phonon calculation. In the lattice structure of graphene, the electrons have a periodic crystal that repeats in space. Thus, calculating a single electron is preferable instead of calculating all the electrons in the system. Furthermore, as it is impossible to calculate infinitely many points in that zone, a set of points known as the K point is decided to sample it.

Graphene is known as a non-magnetic material. In contrast, adding graphene with the other nanomaterials might disturb the spin in the system. This spin polarization observation and the effect on the system can be studied using a spin polarization aspect. Lastly, the basis set modules define the atomic orbitals used for wavefunction expansion, which gives information about the atomic orbitals. Moreover, increasing the basis set size improves the convergence of calculated properties and ensures accurate descriptions of electronic structures.

Here, different simulation software has different operating systems of the DFT components. The comparison of DFT components for each computational software, covering open source and, is presented in Table 2.

Table 2. The typical computational software to calculate DFT

Type	**Name of software**	**Pseudopotentials**	**Exchange-correlation functionals**	**K point sampling**	**Spin polarization**	**Modules**	**Ref.**
Open source	Quantum ESPRESSO	Norm-conserving Pseudopotentials (NCPP) and ultrasoft Pseudopotentials (USPP)	LDA, GGA, and hybrid functionals	Robust K-point sampling for periodic systems	Support spin-polarized calculation	Plane-Wave self-consistent field (PWscf), phonon for phonon, and Car-Parrinello (CP) for molecular dynamic	[15]
	SIESTA		LDA, GGA, and hybrid functionals	Suitable for periodic systems	Support spin-polarized calculation	Molecular dynamic, optical properties, and non-collinear magnetism	[22]

	GPAW	Projector augmented wave (PAW)	LDA, GGA, and hybrid functionals	Robust K-point sampling for periodic systems	Support spin-polarized calculation	Modules for molecular dynamics and optical properties	[23]
Commercial	VASP	USPP and PAW method	LDA, GGA, and hybrid functionals	Efficient K-point sampling for periodic systems	Support spin-polarized calculations for magnetic materials	-	[24]
	CASTEP	NCPP	LDA, GGA, and hybrid functionals	Robust K-point sampling for periodic systems	Supports spin-polarized calculations	Molecular dynamic, phonon calculation, and optical properties	[9]

CHALLENGE AND FUTURE DIRECTIONS

Structural modification of graphene has been widely conducted at the laboratory level, resulting in altered properties. Hybridizing graphene with other nanomaterials has proven to improve potential applications. However, researchers have observed that there are still economic, environmental, and safety concerns associated with the practical implementation. Hence, the computational approach to studying the structure and properties of graphene and its hybrid materials is an alternative solution for studying their further applications.

These potential applications of computational modeling approaches still face some challenges, including functional accuracy, computational cost, defect and doping, and the hybrid system. In some cases, standard exchange-correlation functional such as the LDA and GGA often fail to accurately describe the electronic structure of graphene and its hybrid, particularly in band gap prediction. To overcome these deficits other supported functions are required, such as a strong, constrained, and appropriately normed (SCAN) meta-generalized GGA that shows accuracy and is similar to laboratory results [25]. The incorporation of graphene into other nanomaterials brings further complexity to the interface, such as lattice defects, charge transfer, and interlayer interaction, making it more difficult to predict the structure. The correct simulation of such heterojunctions frequently necessitates multiscale modeling procedures or further than DFT technique, such as many-body perturbation theory, to offer a precise description of the van der Waals force and band alignment [26].

High-fidelity DFT calculations, especially time-dependent DFT (TDDFT), employed to investigate electronic excitations and dynamic phenomena, are computationally costly. These simulations frequently require a high-performance computer (HPC), as a moderate to low level of precursor results in a long execution time. Therefore, there exists a general necessity of generating computationally efficient DFT codes or semi-empirical methods that can be efficiently run on available computing systems without necessarily sacrificing much accuracy. Further research on engineering and dopant integration in graphene is one of the possible directions. DFT studies have the potential to provide important insight into the effect of various dopants, such as B, N, and transition metals, on the electronic structure, carrier concentration, and reactivity of graphene. These insights can be used at the atomic scale as a theory to guide experiments, particularly in sensors, catalysts, and nanoelectronics.

CONCLUSION

Using a computational approach to study graphene and its hybrid materials provides significant advantages, including low cost and the possibility of combining and tailoring the desired application. Based on the previous work, the DFT study on graphene and its hybrid material has been used to investigate its potential for sensing, including gas, lung cancer, and heavy metal sensors. The role of the DFT approach was to facilitate solving the Schrödinger equation to study the quantum behavior of nanomaterials. Both open-source and commercial software can be selected to run the simulation process, including Quantum ESPRESSO, SIESTA, GPAW, VASP, and CASTEP. However, a supercomputer is generally used for complex structures. In view, more student-friendly software and readily accessible computational tools should be developed in order to increase the number of participants involved in this area, including in educational institutions. Moreover, the extension of the DFT methods to medical and biomedical situations can be seen as the direction of future research, which may allow the use of new diagnostic and treatment methods.

DECLARATION OF INTEREST

There is no conflict of interest with this study.

ACKNOWLEDGEMENT

The authors would like to thank Universiti Pendidikan Sultan Idris, Yogyakarta State University, and Diponegoro University for instrumental support.

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