

Graphene-Graphullerene Heterostructure: A Novel Material for High-Performance Capacitors

Anjna Devi^{1,a}, Satish Kumar^{2,b}, Arun Kumar^{2,c}

¹ Government Degree College Baroh, Kangra-176054, Himachal Pradesh, India.

² Government Degree College Bilaspur, Bilaspur-174001, Himachal Pradesh, India.

^a anjnahpu90@gmail.com

^b 97satish02@gmail.com

^c arun242493@yahoo.com

Abstract

This study introduces a novel graphene-graphullerene heterostructure as a promising material for high-performance capacitors. Compared to pristine graphene, this heterostructure exhibits a significantly larger surface area and porosity which enhance its energy storage capacity. Pristine graphullerene is a semiconductor with a bandgap of 0.92 eV and its integration with graphene effectively modifies its electronic properties, rendering it conductive as confirmed by band structure analysis. The unique combination of graphene's high conductivity and graphullerene's extended surface area and porosity presents a promising avenue for developing capacitors with exceptional performance characteristics.

Keywords: DFT, Graphullerene, Electronic Band Structure.

Received 28 January 2025; First Review 02 February 2025; Accepted 07 March 2025

* Address of correspondence

Anjna Devi
Government Degree College Baroh, Kangra-
176054, Himachal Pradesh, India.

Email: anjnahpu90@gmail.com

How to cite this article

Anjna Devi, Satish Kumar, Arun Kumar, Graphene-Graphullerene Heterostructure: A Novel Material for High-Performance Capacitors, J. Cond. Matt. 2025; 03 (01): 38-40.

Available from:
<https://doi.org/10.61343/jcm.v3i01.76>



Introduction

Carbon's diverse bonding allows it to form a variety of structures, such as graphite, diamond, fullerenes, carbon nanotubes, and graphene [1]. These allotropes exhibit a wide range of properties; for instance, diamond is known for its hardness and thermal conductivity, while graphite displays a layered structure and electrical conductivity. Recent research has unveiled novel 2D materials like Graphullerene, a recently synthesized carbon allotrope [2-4]. Graphullerene's unique structure boasts high porosity [3-5] and a significant bandgap, making it a promising candidate for various applications. The integration of Graphullerene with graphene could yield a material with exceptional electrical and surface properties, particularly for energy storage devices such as capacitors. This study explores the Graphene-Graphullerene Heterostructuring (H-Gra/Gph) which leads to high-performance capacitor material.

Method

We conducted density functional theory (DFT) calculations using the SIESTA code [6] to investigate the electronic

properties of the H-Gra/Gph. A GGA-PBE [7] functional and a DZP basis set with a confinement energy of 20 meV were applied. Geometry optimization was performed using the conjugate gradient method with a force tolerance of 0.01 eV/Å, and a 10x10x1 Monkhorst-Pack k-point mesh [8] was used to sample the Brillouin zone. A 15 Å vacuum was applied along the z-axis to minimize interactions between periodic images. Norm-conserving pseudopotentials were employed for all atomic species.

Results and Discussion

The H-Gra/Gph was formed by integrating graphene sheets with graphullerene, creating a composite material with a stable, low-energy configuration. The relaxed hybrid structure of H-Gra/Gph is shown in figure 1(a). The structural optimization of H-Gra/Gph are depicted in Figure 1 (b and c).

Figure 1(b) shows the variation of total energy (E_{Total}) with respect to the lattice constant (a). The plot reveals a well-defined minimum, indicating a stable configuration for the heterostructure at an optimized lattice constant. Figure 1(c) presents the plot of total energy (E_{Total}) versus the vertical

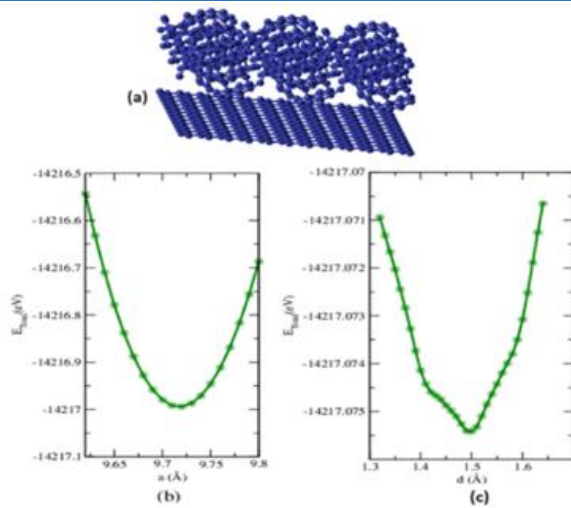


Figure 1: (a) Structure of H-Gra/Gph (b) Lattice constant (a) vs total energy (E_{Total}) plot and (c) vertical separation between Graphene and Graphullerene (d) vs total energy (E_{Total}) plot for H-Gra/Gph.

separation distance (d) between graphene and Graphullerene. This plot also exhibits a clear minimum, suggesting an energetically favourable interlayer distance for the heterostructure. These results provide valuable insights into the structural stability and optimal configuration of the H-Gra/Gph. A comparison of the structural parameters of pure Graphullerene, H-Gra/Gph, and graphene provided in table 1.

Table 1: Optimized lattice constant (a), binding energy (E_b), band gap energy (E_g) of Graphene, Graphullerene and H-Gra/Gph.

Systems	a (Å)	d (Å)	E_b (eV/atom)	E_g (eV)
Graphene	2.49	----	-7.81 (-9.53) ¹²	0.0
Graphullerene	9.32 (9.17) ¹¹	----	-7.44 (-8.564) ⁴	0.92 (I) (0.7 (I)) ⁴
H-Gra/Gph	9.72	1.50	-7.27	----

The lattice constant of the H-Gra/Gph (9.72 Å) is slightly larger than that of pure Graphullerene (9.32 Å), while the binding energy is slightly lower (-7.27 eV/atom compared to -7.44 eV/atom). This suggests that the heterostructure is stable but has a slightly weaker interatomic bonding compared to pure Graphullerene. [4, 9-12].

Figure 2 (a) and (b) shows the electronic band structure and density of states (DOS) of pure Graphullerene and the H-Gra/Gph. Pure Graphullerene exhibits a band gap of approximately 0.92 eV, confirming its semiconducting nature. The DOS plot shows a clear energy gap at the Fermi level supporting this observation. In contrast, the H-Gra/Gph exhibits a metallic behaviour with a zero-band gap. The DOS plot shows a significant overlap of the valence and conduction bands at the Fermi level, indicating the absence of an energy gap. This change in electronic properties is attributed to the interaction between Graphene

and Graphullerene in the heterostructure, which modifies the band structure and leads to the formation of metallic states. Figure 2 (c) and (d) illustrates the density of states (DOS) and integrated density of states (IDOS) for the H-Gra/Gph, pure Graphullerene and Graphene. The prominent peaks in the DOS plots correspond to the electronic states available for charge conduction. The integrated DOS provides a cumulative measure of the number of states up to a given energy level. Comparing the Integrated Density of States (IDOS) plots, we observe that pure Graphullerene exhibits a higher density of states near the Fermi level compared to the H-Gra/Gph. However, it is important to note that capacitance is directly proportional to the density of states at the Fermi level (E_F). While pure Graphullerene may have a higher DOS, the conducting nature of the H-Gra/Gph, along with its porous and large surface area, make it a more promising candidate for electrode materials in supercapacitors.

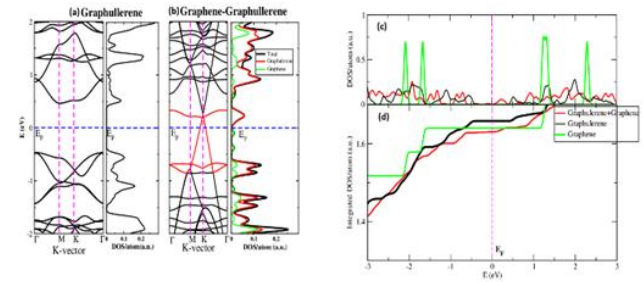


Figure 2: Electronic band structure and density of states of (a) Graphullerene and (b) H-Gra/Gph, (c) Density of states (DOS) and (d) Integrated density of states (IDOS) of H-

Conclusion and Future Prospective

In conclusion, this study has explored the potential of the H-Gra/Gph as a promising material for high-performance capacitors. DFT calculations revealed that the integration of graphene with graphullerene significantly modifies the electronic properties, transforming the semiconducting nature of pure graphullerene into a conductive material. The enhanced conductivity, coupled with the large surface area and porosity of the heterostructure can significantly offers advantages for energy storage applications and more research is needed to synthesises and fabrication processes to fully realize the potential applications of this novel material.

References

1. A. Geim and K Novoselov, Nature Mater, 6,183 (2007).
2. M. A. Khan, M. Atif, M. N. Leuenberger. arXIV 2404.16743. (2024).
3. L. Guang-Ye, M. Shi-Cong, Q. Xin-Yue, N. Jing, L. Jun-Xi, L. Pei-Yi, N. Feng, C. Shi-Zhang, ACS Applied Nano Materials 8(1), 649 (2024).

4. U. Argaman and G. Makov, npj Comp. Mat. 9, 211 (2023).
5. C. Liu, X. Yan, F. Hu, G. Gao, G. Wu, and X. Yang, Adv. Mater 30, e1705713 (2017).
6. J. M. Soler, E. Artacho, J. D. Gale, A. Garcia, J. Junquera, P. Ordejon and D. S. Portal, J. Phys.: Condes. Matter, 14 2745 (2002).
7. J. P. Perdew, K. Burke and M. Ernzerhof, Phys. Rev. Lett, 77:3865 (1996).
8. K. Chaudhary and F. Tavazza Comp. Mater. Sc. 161, 300 (2019).
9. A. Z. Zahran and G. P. Srivastava, App. Surf. Sc. 256 (19), 5783 (2010)
10. A. Devi, A. Kumar, A. Singh and P. K. Ahluwalia, AIP Conf. Proc. 2115, 030386 (2019).
11. S. E. Veras, E. Espada and G. Morell, Carbon Trends 15, 100360 (2024).
12. A. Devi, A. Kumar, P. K. Ahluwalia A. Singh, Materials Science and Engineering: B 271, 115237 (2021).