

# Comparison Study between Borophene/Graphene and Boron-Graphdiyne in DFT using Quantum Espresso

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## Abstract

The global transition from fossil fuels to renewable energy sources under the decarbonization framework raises concerns about energy availability during off-peak periods. To ensure long-term energy storage, battery energy storage systems (BESS) such as sodium-ion batteries (NIBs) have gained significant research attention, particularly regarding their anode materials. This study employs first-principles Density Functional Theory (DFT) calculations using Quantum Espresso to compare the Na adsorption properties of borophene/graphene (B/G) heterostructures and boron-graphdiyne (BGDY) monolayers as potential NIB anode materials. The adsorption energies of Na at three distinct sites were computed based on the total energy of the pristine structures and Na-adsorbed configurations. For the B/G heterostructure, the adsorption energies at sites A, B, and C were 128.6418 eV, 80.2137 eV, and 0.8572 eV, respectively. Meanwhile, the BGDY monolayer exhibited adsorption energies of 2.1973 eV, 2.0681 eV, and 2.8463 eV at the corresponding sites. These values indicate weak or unfavourable Na interactions with both materials, attributed to low charge transfer, weak orbital overlap, unfavourable adsorption geometries, and unoptimized structures. Consequently, neither material is currently suitable for NIB applications without further modification. Future research should focus on structural optimization and surface modifications to achieve negative adsorption energies, enabling a more comprehensive comparison of their potential as anode materials.

## 1. Introduction

Energy plays a crucial role in modern society, driving advancements and shaping daily life. The global transition from fossil fuels to renewable energy sources has heightened the need for efficient energy storage systems (ESS) [1]. Among various energy storage technologies, sodium-ion batteries (NIBs) have emerged as a promising alternative to lithium-ion batteries (LIBs) due to the abundance, low cost, and environmental benefits of sodium [2]. Sodium, the fourth most abundant element in the Earth's crust, offers a sustainable and scalable solution for large-scale energy storage applications [3]. However, challenges such as the larger ionic radius of sodium compared to lithium, unstable electrochemical performance, and insufficient energy capacities hinder the commercialization of NIBs [4]. Addressing these limitations requires the development of advanced anode materials with superior conductivity, reversibility, cycling stability, and high specific capacity [5].

Two-dimensional (2D) materials have gained attention as potential anode materials due to their unique structural and electronic properties [6]. They provide high surface-to-volume ratios, multiple adsorption sites for

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Na-ion storage, and a smooth surface geometry that lowers diffusion barriers, enabling faster charge-discharge rates and improved cyclic stability [7]. Among 2D materials, carbon-based structures such as graphene have been widely studied due to their high electrical conductivity and mechanical strength [8]. Despite its excellent properties, pristine graphene has a zero bandgap and weak Na adsorption, which limits its effectiveness as an anode material [9]. To overcome this issue, heteroatom doping and heterostructure engineering have been explored to enhance sodium storage performance [10]. Borophene, a 2D boron lattice, exhibits high conductivity and ultrahigh theoretical capacity, making it a strong candidate for NIB anodes [11]. Studies by Zhang et al. demonstrated that borophene phases such as  $\beta_{12}$  and  $\chi^3$  enhance the power density and diffusion rates of NIBs [12]. Meanwhile, boron-doped graphdiyne (BGDY) has been proposed as an alternative due to its tunable electronic properties and potential for improved Na-ion storage [13]. However, a comprehensive theoretical comparison between borophene/graphene (B/G) heterostructures and BGDY monolayers as NIB anode materials is still lacking.

Computational studies play a crucial role in understanding material properties at the atomic level, guiding experimental efforts toward optimizing battery performance. Density Functional Theory (DFT), a widely used first-principles approach, provides insights into the electronic structure, charge transfer mechanisms, and adsorption energies of materials [14]. Quantum Espresso, an open-source DFT-based software package, is particularly well-suited for this type of study due to its efficient handling of plane-wave basis sets, pseudopotential methods, and ability to model complex material interactions [15]. Previous studies have successfully employed Quantum Espresso to investigate adsorption properties in 2D materials, providing accurate predictions that align with experimental findings [16].

In this study, first-principles calculations using DFT within the Quantum Espresso framework are employed to compare the Na adsorption properties of B/G heterostructures and BGDY monolayers. The total energy of pristine structures and Na-adsorbed configurations at three different adsorption sites is computed to evaluate adsorption energies. This investigation aims to provide a theoretical understanding of Na-ion interactions with these materials, analysing their adsorption behaviour through configurated total energy and calculated adsorption energies. The results of this study contribute to the ongoing search for high-performance anode materials, helping to identify structural advantages and limitations in 2D materials for sodium-ion battery applications. By evaluating adsorption characteristics, this research aims to guide future advancements in optimizing structural modifications and electronic properties of anode materials to enhance their electrochemical performance, thereby facilitating the commercial viability of NIBs as a sustainable alternative to LIBs.

## 2. Research Methodology

The adsorption of sodium (Na) atoms at three distinct sites (A, B, C) on both the boron-doped graphdiyne (BGDY) monolayer and the borophene/graphene (B/G) heterostructure was investigated using Density Functional Theory (DFT) as implemented in the Quantum Espresso package. Quantum Espresso is a widely used open-source software suite for electronic-structure calculations and materials modelling, based on plane-wave basis sets and pseudopotentials [15].

The Perdew-Burke-Ernzerhof (PBE) functional within the Generalized Gradient Approximation (GGA) was employed to describe electron exchange-correlation effects, which has been validated for structural and energetic predictions in similar materials [16]. To address partial electronic occupancies arising from the metallic nature of the systems, Marzari-Vanderbilt smearing was applied with a width of 0.01 Ry for BGDY and 0.02 Ry for B/G [17].

For the BGDY monolayer, van der Waals (vdW) interactions were accounted for using the Grimme-D3 correction, which has been demonstrated to improve the accuracy of long-range dispersion interactions in layered materials [18]. The interaction between valence electrons and ionic cores was described using projector augmented wave (PAW) pseudopotentials from the Standard Solid-State Pseudopotentials (SSSP) library, ensuring an accurate electronic structure representation [19].

A plane-wave kinetic energy cutoff of 44 Ry and a charge density cutoff of 240 Ry were set, with the Brillouin zone sampled using a Monkhorst-Pack grid of  $9 \times 9 \times 1$  k-points. The BGDY monolayer was optimized to a lattice constant of 11.8 Å, with convergence thresholds of  $10^{-5}$  Ry for total energy and  $10^{-8}$  Ry for the self-consistent field (SCF) calculations [20].

For the B/G heterostructure, a supercell was constructed by layering a  $3 \times 3$  borophene monolayer onto a  $2 \times 2$  graphene monolayer, resulting in a 4.2% lattice mismatch with a lattice constant of  $a = b = 4.92081$  Å. The borophene layer was positioned 4 Å above the graphene layer, with interlayer distances ranging from 3.8 to 4.9 Å. An  $8 \times 8 \times 1$  Monkhorst-Pack grid was employed, and the plane-wave kinetic energy cutoff was set to 500 eV. The convergence criteria for forces and total energy were set to  $10^{-3}$  Ry/Bohr and  $10^{-6}$  Ry, respectively [21].

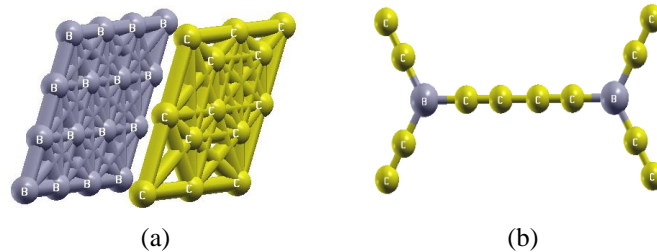
These computational parameters are consistent with established practices in modelling 2D heterostructures, ensuring accuracy and reliability [22]. By following validated computational methodologies, this study aims to provide reliable insights into the Na adsorption properties of BGDY monolayers and B/G heterostructures, contributing to the development of efficient anode materials for sodium-ion batteries (NIBs).

The adsorption energy ( $E_{ads}$ ) was calculated as

$$(E_{ads}) = E_{Total\ energy} - (E_{Adsorbed} + E_{Isolated\ Na\ atom}) \quad (1)$$

### 3. Result and Discussion

#### 3.1 Total Energy Of Pristine Structure



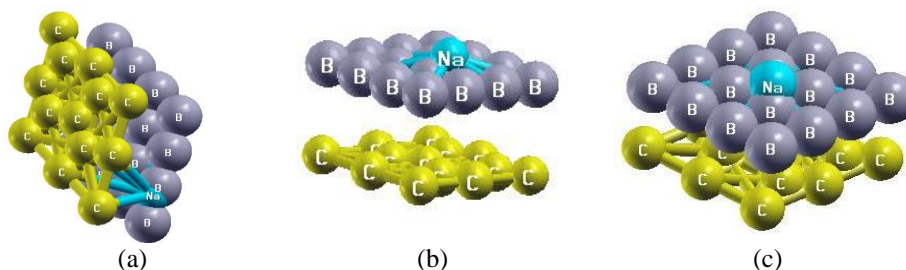
**Fig. 1** (a) Pristine B/G Heterostructure; (b) BGDY monolayer

The pristine structures of borophene and graphene were optimized using SCF calculations, with initial input geometries specified in pw.x format. The borophene layer, characterized by triangular and hexagonal motifs, was stacked with the graphene layer, forming a heterostructure (B/G) as shown in Fig. 1. The pristine B/G heterostructure displayed a C-C bond length of 1.42 Å, while the B-B bond lengths in the borophene layer ranged from 1.64 Å to 1.89 Å. Interlayer distances were set to 4.9 Å (maximum) and 3.8 Å (minimum), allowing sufficient space for sodium (Na) intercalation [23]. The optimized lattice constants were 4.92 Å for the B/G heterostructure and 11.8 Å for the BGDY monolayer, consistent with earlier reports on similar systems [20]. Based on the geometry optimization, the final energy for B/G heterostructure is -155.7069Ry and -243.3368 for BGDY as per Table 1.

**Table 1** Total energy of pristine structure

Pristine Structure	Total Energy (Ry)	Total Energy (eV)
BGDY	-243.3368	-3310.7658
B/G	-155.7069	-2118.5003

#### 3.2 Total energy of adsorption sites of B/G



**Fig. 2** (a) Site A (Lower/bridge-like), (b) Site B (hollow site), (c) Site C (Alternate top)

The total energy values after introducing sodium (Na) adsorption on the Borophene/Graphene (B/G) heterostructure are -3296.9084 eV at Site A (Lower/Bridge-like), -3345.3365 eV at Site B (Hollow site), and -3438.2988 eV at Site C (Alternate top site). Based on the results indicate that Site A, with the lowest total energy, is the most energetically favourable for Na adsorption, followed by Site B and then Site C. In density functional theory (DFT) studies, lower total energy values correspond to more stable adsorption sites. Therefore, Na adsorption is most favourable at Site A and least favourable at Site C.

The stability at Site A can be attributed to the enhanced coordination between Na and both boron (B) and carbon (C) atoms. The bridge-like structure allows for increased charge transfer, stabilizing Na through delocalized interactions across multiple atomic sites. This phenomenon is consistent with previous studies on

borophene based materials, which indicate that adsorption stability is highest at bridge sites due to stronger electrostatic and covalent contributions [24]. Site B (Hollow site) is the second most stable adsorption site, as indicated by its intermediate total energy. The hollow site typically provides a high coordination number, where Na is stabilized by interactions with multiple surrounding boron atoms rather than a single adsorption center. This effect has been reported in studies of Na adsorption on two-dimensional materials, where hollow sites generally provide strong adsorption due to increased electron density and enhanced binding interactions [25].

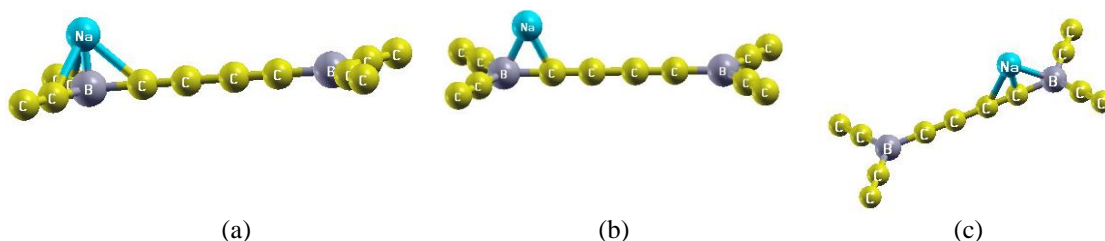
Conversely, Site C (Alternate Top site) is the least favourable adsorption site, as indicated by the highest energy value of -3438.2988 eV. The positioning of Na directly above a single boron atom leads to low coordination and weak binding, reducing adsorption stability. The absence of multiple interacting atoms results in higher electrostatic repulsion and limited charge transfer, making the adsorption process less energetically favourable. This observation is consistent with findings on Na adsorption in borophene and graphene heterostructures, where adsorption at top sites often results in weak interactions due to the lack of multi-atomic coordination [26].

The stability of Na adsorption in the B/G heterostructure follows a stability trend of Site A > Site B > Site C, where bridge-like adsorption sites offer the most favourable interactions due to their enhanced charge transfer properties, while top sites are least favourable due to weak bonding and electrostatic repulsion

**Table 2** Total energy of adsorption sites of B/G

Adsorption sites	Total Energy (Ry)	Total Energy (eV)
A	-242.3183	-3296.9084
B	-245.8777	-3345.3365
C	-252.7103	-3438.2988

### 3.3 Total energy of adsorption sites of BGDY



**Fig. 3** (a) Site A (Above B); (b) Site B (Bridge Between B and C1); (c) Site C (Bridge Between B and C2)

From Table 3 computed total energies for these configurations were -352.3227 Ry (-4793.5944 eV), -352.3322 Ry (-4793.7237 eV), and -352.2750 Ry (-4792.9455 eV) for Sites A, B, and C, respectively. Based on these values, Site B exhibits the highest stability, followed by Site A, while Site C is the least stable.

The preference for the bridge adsorption site (B-C1) over the top site (B) and the alternative bridge site (B-C2) was attributed to optimized charge redistribution and stronger bonding interactions between Na, B, and C atoms. Prior computational studies have suggested that alkali metal atoms, such as Na, prefer bridge adsorption sites due to enhanced charge transfer and electronic stability, reducing overall system energy [27], [28]. A study [27] confirmed that boron-doped graphdiyne exhibits strong Na adsorption, making it a potential candidate for sodium-ion batteries (NIBs). Similarly, research by [28] highlighted that the presence of boron improves the adsorption and diffusion properties of Na, leading to improved anode performance. The least stable configuration at Site C indicates weaker binding interactions, which could lead to increased Na mobility and lower adsorption efficiency, as also observed in studies focusing on boron-doped graphene [29].

The trend aligns with previous DFT-based investigations on alkali metal interactions with carbon-based materials, where bridge sites are often favoured over top or hollow sites due to their optimal adsorption energy and structural stability. Additionally, boron doping plays a crucial role in modifying the electronic environment of graphdiyne, enhancing its capacity to accommodate Na atoms, thereby influencing sodium-ion battery (NIB) anode performance [27], [29].

**Table 3** Total energy of adsorption sites of B/G

Adsorption sites	Total Energy (Ry)	Total Energy (eV)
A	-352.3227	-4793.5944
B	-352.3322	-4793.7237
C	-352.2750	-4792.9455

### 3.4 Adsorption energy

The adsorption energy values for sodium (Na) at three different sites in both the borophene/graphene (B/G) heterostructure and boron-doped graphdiyne (BGDY) monolayer were found to be large and positive, indicating endothermic interactions. This suggests that Na adsorption on both structures is thermodynamically unfavorable. The geometries at these sites were not optimized due to the extended duration of the calculations and failure to achieve convergence. These unrelaxed geometries likely resulted in higher energy values. Furthermore, inaccuracies in the choice of input parameters for the self-consistent field (SCF) calculation may have contributed to the large positive adsorption energies, as previously noted in computational studies on sodium-ion interactions with carbon-based materials [27].

Both the B/G heterostructure and BGDY monolayer exhibit significant challenges with Na adsorption, likely due to inherent structural strain. The B/G heterostructure has a lattice mismatch of 4.2% between borophene and graphene layers, causing structural distortions upon Na introduction. This strain is exacerbated by Na's interaction with the surface, preventing the system from reaching a stable configuration during relaxation. Similarly, in the BGDY monolayer, the positioning of Na at sites A, B, and C creates unfavourable geometries that hinder the relaxation process, preventing convergence. These issues indicate that the potential energy surfaces (PES) for Na adsorption on both materials lack well-defined local minima, preventing stable Na adsorption, as also observed in studies of alkali metal adsorption on boron-doped carbon materials [27].

The weak adsorption behaviour can be attributed to the electronic structure of both materials. The delocalized  $\pi$ -electrons in the B/G heterostructure, while favourable for conductivity, do not form strong interactions with Na's partially filled 3s-orbital. The metallic or semi-metallic character of borophene inhibits charge transfer, leading to weak or repulsive bonding interactions. Similarly, the BGDY monolayer, with its  $sp^2$  hybridization and acetylenic linkages, provides insufficient bonding sites for Na, resulting in low charge transfer and poor orbital overlap. The lack of significant van der Waals interactions in both structures further contributes to the large positive adsorption energies [29].

For comparison, the adsorption energy of Na at Site A of the BGDY monolayer was found to be 2.1973 eV, significantly larger than the value of -1.22 eV reported by Muhammad et al. [20]. This discrepancy may stem from differences in Na's position and the parameters used in the calculations. The input files for BGDY were manually generated, which may have introduced inconsistencies in atomic positions. For the B/G heterostructure, the absence of reference input files led to variations in atomic positions, making the geometry optimization more complex and time-consuming, which further prevented convergence.

Optimizing the input files and atomic configurations for both structures is crucial to improving the accuracy of adsorption energy calculations. With proper optimization, the study could proceed with further calculations, such as diffusion energy, specific capacity, and open-circuit voltage, and could investigate the trend in adsorption with increasing Na concentration. Additionally, optimizing the BGDY bilayer and comparing it with the B/G heterostructure could provide further insights into their adsorption properties. Prior studies suggest that a bilayer structure may help stabilize Na adsorption by increasing interlayer interactions, thereby enhancing sodium-ion storage efficiency [30].

Due to the unavailability of input files and the challenges in determining the atomic positions of Na, the adsorption energy values could have been large and positive values. Addressing these limitations and optimizing the structures will be necessary for advancing the study of potential anode materials for sodium-ion batteries (NIBs). Further refinement of computational methodologies, including hybrid functionals and van der Waals corrections, could provide more reliable adsorption energy predictions, as demonstrated in previous density functional theory (DFT) studies on alkali metal storage materials [31].

**Table 4** Adsorption energy

Structure	Adsorption energy (eV)		
	A	B	C
B/G	128.6418	80.2137	0.8572
BGDY	2.1973	2.0681	2.8463

#### 4. Conclusion

This study aimed to perform DFT calculations in Quantum Espresso to determine Na adsorption energy for Borophene/Graphene (B/G) heterostructures and Boron Graphdiyne (BGDY) monolayers across three different adsorption sites. The goal was to assess their suitability as anode materials for sodium-ion batteries (NIBs). The adsorption energy values for the B/G heterostructure at sites A, B, and C were 128.6418eV, 80.2137eV, and 0.8572eV, respectively. These large positive values indicate that Na exhibits weak interactions with the B/G substrate, making adsorption energetically unfavourable across all sites. The high adsorption energies at sites A and B suggest strong repulsion between Na and B/G, while site C shows a lower value, though still deviating from the expected range for stable adsorption. In the BGDY monolayer, the adsorption energy values at sites A, B, and C were 2.1973eV, 2.0681eV, and 2.8463eV, respectively. While these values are lower than those in B/G, they remain positive, indicating weak interactions between Na and the BGDY surface.

The observed large adsorption energies can be attributed to weak charge transfer, minimal orbital overlap, and unfavourable adsorption geometries, which prevent strong Na binding. The intrinsic strain in the B/G heterostructure further weakens interactions, while the rigid structure of BGDY restricts adsorption flexibility. These factors suggest that both materials require further modifications to improve their potential as anode materials. Future work should focus on optimizing atomic positions, introducing dopants or functional groups to enhance charge transfer, and exploring bilayer or multilayer configurations for better Na stabilization. Additional computational analyses such as diffusion energy and electronic structure calculations could provide deeper insights into Na storage behaviour. Comparing results with experimental data will also help validate computational predictions and refine the methodology.

Although the Na adsorption energy values deviate significantly from the desired range for effective NIB anode materials, these results serve as a foundation for further material tuning and structural optimization. Implementing advanced structural modifications and computational improvements will be essential in developing a more comprehensive understanding of Na-ion storage mechanisms in these materials.

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#### Conflict of Interest

Authors declare that there is no conflict of interests regarding the publication of the paper.

#### Author Contribution

The authors confirm contribution to the paper as follows: **study conception and design:** Visrutii Ramess; **data collection:** Visrutii Ramess; **analysis and interpretation of results:** Visrutii Ramess, *Ahmad Hassan Sallehudin Mohd Sarif*; **draft manuscript preparation:** Visrutii Ramess, *Ahmad Hassan Sallehudin Mohd Sarif*. All authors reviewed the results and approved the final version of the manuscript.

#### References

- [1] D. Larcher and J.-M. Tarascon, "Towards greener and more sustainable batteries for electrical energy storage," *Nat Chem*, vol. 7, no. 1, pp. 19–29, Jan. 2015, doi: 10.1038/nchem.2085.
- [2] M. H. Han, E. Gonzalo, G. Singh, and T. Rojo, "A comprehensive review of sodium layered oxides: powerful cathodes for Na-ion batteries," *Energy Environ Sci*, vol. 8, no. 1, pp. 81–102, 2015, doi: 10.1039/C4EE03192J.
- [3] S. Kim, D. Seo, X. Ma, G. Ceder, and K. Kang, "Electrode Materials for Rechargeable Sodium-Ion Batteries: Potential Alternatives to Current Lithium-Ion Batteries," *Adv Energy Mater*, vol. 2, no. 7, pp. 710–721, Jul. 2012, doi: 10.1002/aenm.201200026.
- [4] M. D. Slater, D. Kim, E. Lee, and C. S. Johnson, "Sodium-Ion Batteries," *Adv Funct Mater*, vol. 23, no. 8, pp. 947–958, Feb. 2013, doi: 10.1002/adfm.201200691.
- [5] C. Vaalma, D. Buchholz, M. Weil, and S. Passerini, "A cost and resource analysis of sodium-ion batteries," *Nat Rev Mater*, vol. 3, no. 4, p. 18013, Mar. 2018, doi: 10.1038/natrevmats.2018.13.
- [6] M. Pasta, C. D. Wessells, R. A. Huggins, and Y. Cui, "A high-rate and long cycle life aqueous electrolyte battery for grid-scale energy storage," *Nat Commun*, vol. 3, no. 1, p. 1149, Oct. 2012, doi: 10.1038/ncomms2139.
- [7] H. Kim, J. Hong, Y. Park, J. Kim, I. Hwang, and K. Kang, "Energy Storage: Sodium Storage Behavior in Natural Graphite using Ether-based Electrolyte Systems (*Adv. Funct. Mater.* 4/2015)," *Adv Funct Mater*, vol. 25, no. 4, pp. 652–652, Jan. 2015, doi: 10.1002/adfm.201570029.
- [8] A. K. Geim and K. S. Novoselov, "The rise of graphene," *Nat Mater*, vol. 6, no. 3, pp. 183–191, Mar. 2007, doi: 10.1038/nmat1849.

- [9] M. Pumera, A. Ambrosi, A. Bonanni, E. L. K. Chng, and H. L. Poh, "Graphene for electrochemical sensing and biosensing," *TrAC Trends in Analytical Chemistry*, vol. 29, no. 9, pp. 954–965, Oct. 2010, doi: 10.1016/j.trac.2010.05.011.
- [10] L. Zhang, Z. Chou, H. Zhang, X. Wang, and X. Xiao, "Improving sodium ion storage performance by heteroatom strategy with nitrogen and sulfur doping carbon sheets," *J Energy Storage*, vol. 111, p. 115412, Mar. 2025, doi: 10.1016/j.est.2025.115412.
- [11] X. Zhang, J. Hu, Y. Cheng, H. Y. Yang, Y. Yao, and S. A. Yang, "Borophene as an extremely high capacity electrode material for Li-ion and Na-ion batteries," *Nanoscale*, vol. 8, no. 33, pp. 15340–15347, 2016, doi: 10.1039/C6NR04186H.
- [12] B. Mortazavi, A. Dianat, O. Rahaman, G. Cuniberti, and T. Rabczuk, "Borophene as an anode material for Ca, Mg, Na or Li ion storage: A first-principle study," *J Power Sources*, vol. 329, pp. 456–461, Oct. 2016, doi: 10.1016/j.jpowsour.2016.08.109.
- [13] H. Zhang et al., "Graphdiyne: A promising anode material for lithium ion batteries with high capacity and rate capability," *J Appl Phys*, vol. 113, no. 4, Jan. 2013, doi: 10.1063/1.4789635.
- [14] P. Hohenberg and W. Kohn, "Inhomogeneous electron gas," *Physical Review*, vol. 136, no. 3B, 1964, doi: 10.1103/PHYSREV.136.B864/FIGURE/1/THUMB.
- [15] P. Giannozzi et al., "QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials," *Journal of Physics: Condensed Matter*, vol. 21, no. 39, p. 395502, Sep. 2009, doi: 10.1088/0953-8984/21/39/395502.
- [16] J. P. Perdew, K. Burke, and M. Ernzerhof, "Generalized Gradient Approximation Made Simple," *Phys Rev Lett*, vol. 77, no. 18, pp. 3865–3868, 1996, doi: 10.1103/PhysRevLett.77.3865.
- [17] N. Marzari, D. Vanderbilt, A. De Vita, and M. C. Payne, "Thermal Contraction and Disorder of the Al(110) Surface," *Phys Rev Lett*, vol. 82, no. 16, pp. 3296–3299, 1999, doi: 10.1103/PhysRevLett.82.3296.
- [18] S. Grimme, "Semiempirical GGA-type density functional constructed with a long-range dispersion correction," *J Comput Chem*, vol. 27, no. 15, pp. 1787–1799, Nov. 2006, doi: 10.1002/JCC.20495.
- [19] K. Lejaeghere et al., "Reproducibility in density functional theory calculations of solids," *Science*, vol. 351, no. 6280, Mar. 2016, doi: 10.1126/SCIENCE.AAD3000.
- [20] I. Muhammad, S. Wang, J. Liu, H. Xie, and Q. Sun, "Boron-graphdiyne as an anode material for Li, Na, and K ion batteries with high capacities and low diffusion barriers," *Journal of Renewable and Sustainable Energy*, vol. 11, no. 1, Jan. 2019, doi: 10.1063/1.5079928.
- [21] F. Ahmad, T. Alkori, and H. Alatas, "DFT Study of Borophene/Graphene (B/G) Heterostructure Properties as Sodium-Ion Battery Anode," 2023.
- [22] H. J. Monkhorst and J. D. Pack, "Special points for Brillouin-zone integrations," *Phys Rev B*, vol. 13, no. 12, pp. 5188–5192, 1976, doi: 10.1103/PhysRevB.13.5188.
- [23] F. Ahmad, T. Alkori, and H. Alatas, "DFT Study of Borophene/Graphene (B/G) Heterostructure Properties as Sodium-Ion Battery Anode," 2023.
- [24] J. Liu, C. Zhang, L. Xu, and S. Ju, "Borophene as a promising anode material for sodium-ion batteries with high capacity and high rate capability using DFT," *RSC Adv*, vol. 8, no. 32, pp. 17773–17785, May 2018, doi: 10.1039/C8RA01942H.
- [25] L. Shi, T. Zhao, A. Xu, and J. Xu, "Ab initio prediction of borophene as an extraordinary anode material exhibiting ultrafast directional sodium diffusion for sodium-based batteries," *Science Bulletin* 2016 61:14, vol. 61, no. 14, pp. 1138–1144, Jun. 2016, doi: 10.1007/S11434-016-1118-7.
- [26] J. Fan, H. Chen, and X. Niu, "Unraveling the enhanced sodium-storage mechanism in a strongly bonded 2D honeycomb borophene/boron phosphide heterostructure," *Appl Phys Lett*, vol. 125, no. 14, Sep. 2024, doi: 10.1063/5.0224095/3315071.
- [27] S. Gharehzadeh Shirazi, M. Nasrollahpour, and M. Vafaei, "Investigation of Boron-Doped Graphdiyne as a Promising Anode Material for Sodium-Ion Batteries: A Computational Study," *ACS Omega*, vol. 5, no. 17, pp. 10034–10041, May 2020, doi: 10.1021/acsomega.0c00422.
- [28] M. Nasrollahpour, M. Vafaei, M. R. Hosseini, and H. Irvani, "Ab initio study of sodium diffusion and adsorption on boron-doped graphyne as promising anode material in sodium-ion batteries," *Physical Chemistry Chemical Physics*, vol. 20, no. 47, pp. 29889–29895, Dec. 2018, doi: 10.1039/C8CP04088E.
- [29] M. S. Ritopečki, N. V. Skorodumova, A. S. Dobrota, and I. A. Pašti, "Boron-doped graphene -- DFT study of the role of dopant concentration and oxidation on sodium and aluminium storage applications," Jul. 2023, Accessed: Jan. 20, 2025. [Online]. Available: <https://arxiv.org/abs/2307.02885v1>
- [30] K. S. Novoselov et al., "Two-dimensional gas of massless Dirac fermions in graphene," *Nature*, vol. 438, no. 7065, pp. 197–200, Nov. 2005, doi: 10.1038/NATURE04233.
- [31] H. Zhang et al., "Ions and electrons dual transport channels regulated by nanocellulose for mitigating dendrite growth of zinc-ion batteries," *Chemical Engineering Journal*, vol. 505, p. 159476, Feb. 2025, doi: 10.1016/J.CEJ.2025.159476.