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Research Paper

Adsorptions of Sodium Ion/Atom on Graphene Quantum Dots for Battery Applications: A DFT Study

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Abstract

Sodium-ion batteries (SIBs) are emerging as a cost-effective and sustainable alternative to lithium-ion batteries, yet they face challenges such as lower energy density and electrode material instability. This study explores the potential of coronene and circumcoronene-based graphene quantum dots (GQDs) as anode materials for SIBs, focusing on three adsorption areas: central, intermediate, and edge, under two battery conditions: charging and discharging. By addressing these limitations through advanced nanostructuring, we employed density functional theory (DFT) with the M06-2X/6-31G+(d) level of theory to conduct comprehensive analyses of sodium adsorption on GQDs. Our findings reveal that both coronene and circumcoronene GQDs preferentially adsorb sodium at the edge areas due to the highest energy adsorption. In discharging conditions, coronene exhibited an adsorption energy of -1.09 kcal/mol, while circumcoronene showed -9.84 kcal/mol. In charging conditions, the adsorption energies were -33.44 kcal/mol for coronene and -37.19 kcal/mol for circumcoronene. Additionally, the energy gap of GQDs was significantly reduced after sodium adsorption, from 5.84 eV to 1.38 eV for coronene and from 4.33 eV to 1.63 eV for circumcoronene. Both GQDs showed theoretical voltages in the range of 1.40 to 1.47 V for coronene and 1.19 to 1.22 V for circumcoronene, respectively. Conclusively, our study recommends circumcoronene as large-sized GQDs as optimal SIB anode materials, offering higher adsorption energy, good conductivity, and reasonable electrochemical performance. This research addresses a theoretical gap by illuminating the impact of Na adsorption on GQD molecular and electronic structures, aiding in the design of enhanced capacity nano-anodes for SIBs.

Keywords
DFT, Sodium-Ion Batteries, Sodium Adsorption, GQDs, Energy Storage

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1. INTRODUCTION

Sodium-ion batteries (SIBs) are gaining attention as a promising alternative to lithium-ion batteries due to the abundance and cost-effectiveness of sodium. This transition is crucial for achieving the United Nations' Sustainable Development Goal 7 (SDG 7), which focuses on ensuring access to affordable, reliable, sustainable, and modern energy for all (Hannan et al., 2021; Wanison et al., 2024). SIBs offer several advantages, including reduced costs, enhanced thermal stability, faster charging capabilities, and improved safety profiles compared to lithium-ion batteries (Hwang et al., 2017; Kim, 2023; Tarascon, 2020). Despite their advantages, sodium-ion batteries (SIBs) face significant challenges, including lower energy density, shorter cycle life, and electrode material instability (Cai et al., 2024; Nithya and Gopukumar, 2015; Sada et al., 2023). These issues are primarily due to the larger size of sodium ions compared to lithium ions (Nayak et al., 2018; Zhao et al., 2023). Additionally, the development of compatible electrolytes and the establishment of robust industrial supply chains remain critical hurdles. For instance, the current energy density of SIBs is approximately 150 Wh/kg, which is lower than that of lithium-ion batteries (Xu et al., 2023).

Advancements in nanotechnology and nanomaterials provide promising solutions to the challenges faced by energy storage systems (Almafie et al., 2024; Mahmud, 2023; Ong et al., 2021). Nanostructured materials such as graphene quantum dots (GQDs), nanowires, and nanotubes increase surface area and offer more active sites for sodium ion adsorption, thereby enhancing energy density (Dave and Gomes, 2019; Wen et al., 2024). GQDs, nanoscale fragments of graphene, are particularly promising due to their exceptional electronic and physicochemical properties. Their high surface area, excellent conductivity, and abundant active sites significantly improve the electrochemical performance of energy storage devices, including supercapacitors and lithium-sulfur batteries (Liu et al., 2020). Experimental studies have shown that GQDs significantly enhance anode performance in metal-ion batteries (Puttaswamy et al., 2022; Shaker et al., 2023). The high surface area, excellent conductivity, and abundant active sites of GQDs contribute to reducing volume expansion and promoting electron transfer and ion diffusion (Yan et al., 2019). Theoretical studies using density functional theory (DFT) are essential for optimizing graphene quantum dots (GQDs) in battery applications (Bekeur and Mapasha, 2023; Daryabari et al., 2021; Saadh et al., 2024). Coronene and circumcoronene are widely used models for graphene quantum dots (GQDs) due to their structural and electronic resemblance to larger graphene sheets. As polycyclic aromatic hydrocarbons (PAHs), they capture the essential hexagonal carbon lattice of graphene, making them ideal for studying electronic properties using density functional theory (DFT). Their size ensures computational feasibility while highlighting crucial edge effects that influence adsorption and conductivity (Budyka, 2019; Malček and Cordeiro, 2018). Compared to smaller PAHs like naphthalene and anthracene, which offer limited π-conjugation, and phenanthrene and tetracene, which lack the necessary size and complexity, coronene and circumcoronene provide a more accurate representation of graphene's extended electronic properties. Although larger molecules like ovalene and hexabenzocoronene offer closer approximations, they are computationally more demanding (Paternò et al., 2021; Shi et al., 2019a; Shi et al., 2019b). Coronene, with its seven-ring structure, and circumcoronene, with its even larger framework, strike a balance between computational feasibility and structural accuracy, providing sufficient π-conjugation to effectively model graphene's electronic properties. These molecules are well-documented in the literature as reliable models for GQDs, offering a robust foundation for extrapolating findings to larger graphene systems (Santa Daría et al., 2024). Their well-documented electronic properties, including band gap variations, are essential for tailoring GQDs for applications in energy storage and electronics (Geetha Sadasivan Nair et al., 2024; Malček et al., 2018).

DFT provides insights into ion adsorption and diffusion, predicts electronic structures and binding energies, and evaluates material performance before synthesis (Mulya and Parasuk, 2020). It guides experiments by identifying promising materials and configurations, saving time and resources. Additionally, DFT explores modifications like doping or functionalization to enhance conductivity and stability. By combining DFT insights with experimental findings, researchers can develop more efficient and sustainable SIBs, advancing energy storage solutions.

Addressing a crucial gap in the research on sodium-ion batteries (SIBs), this study investigates the potential of coronene and circumcoronene-based graphene quantum dots (GQDs) as anode materials. While a few researchers have focused on the use of GQDs in energy storage, there is a lack of research specifically concerned with their application in SIBs. Therefore, this research focuses on theoretical voltage calculations, adsorption energy analysis, and the impact of sodium adsorption on the energy gap of these materials. By leveraging the unique properties of GQDs, this study aims to address the current limitations of SIBs and contribute to the development of more efficient, sustainable, and cost-effective energy storage solutions. Through our analysis, we provide valuable insights into the design of advanced anode materials for SIBs, enhancing their performance and viability.

2. EXPERIMENTAL SECTION

Coronene ($C_{24}H_{12}$) and circumcoronene ($C_{54}H_{18}$) were used as models for hexagonal-shaped graphene quantum dots (GQDs). Sodium ion and atom were considered adsorbed on hollow sites. Adsorption zones are categorized as central, intermediate, and edge, marked by color: blue for central, green for intermediate, and yellow for edge, as shown in Figure 1, following a previous study by Alonso-Lanza et al. (2017).

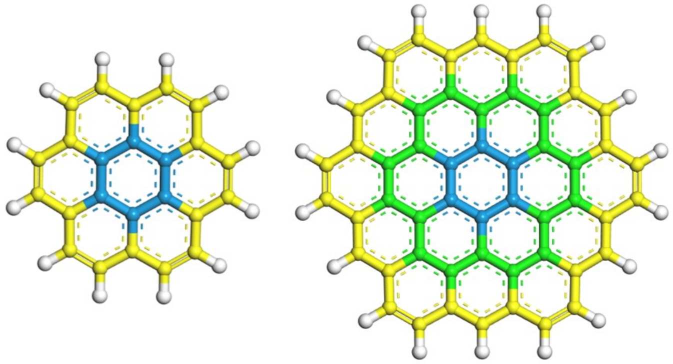

Figure 1. Coronene and Circumcoronene GQDS, Classified Based on The Area: Central Area (Blue), Intermediate Area (Green) and Edge Area (Yellow)

Density functional theory (DFT) calculations utilizing hybrid meta exchange-correlation functional M06-2X and 6-31G+(d) basis set were performed to explore the interaction of sodium ions with graphene quantum dots (GQDs) derived from coronene and circumcoronene. The M06-2X was chosen for this study because of its balanced treatment of exchange-correlation interactions and its proven capability to accurately model non-covalent interactions and dispersion effects (Zhao and Truhlar, 2008). However, it is important to note that while M06-2X is effective for non-covalent interactions, it may have limitations in modeling larger systems or certain types of electronic transitions. The 6-31G+(d) basis set was chosen for its computational efficiency and accuracy in capturing the electronic properties of GQDs. The study focused on the sodium ion adsorption at various sites on the GQDs, specifically central, edge, and intermediate positions on circumcoronene-based

GQDs, and central and edge positions on coronene-based GQDs. All calculations were conducted at room temperature and ambient pressure using Gaussian16 software (Lipparini et al., 2016). Optimized structures were analyzed to obtain key electronic properties such as the highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) energy, and the total energies of each configuration. Furthermore, the adsorption energy were calculated to assess the interaction strength between the sodium atom/ion and the GQD surfaces. Adsorption energy was computed using the formula:

$$E_{\text{ads}} = E_{\text{GQDs+Na}} - E_{\text{GQDs}} - E_{\text{Na}} \tag{1}$$

Additionally, the energy gap (E_g) was determined from the difference between the LUMO and HOMO energies:

$$E_g = E_{\text{LUMO}} - E_{\text{HOMO}} \tag{2}$$

These computational analyses are crucial for understanding the electronic properties of GQDs when interfaced with sodium ions, offering valuable insights into their potential applications in sodium-ion batteries.

Table 1. Adsorptions Energies (Kcal/Mol), HOMO, LUMO, and Gap Energies (Ev) of Coronene and Circumcoronene at The Central (C), Intermediate (I) and Edge (E) Locations

GQDs model	E_{Ads}	E_{HOMO}	E_{LUMO}	E_g
Na-$C_{24}H_{12}$-C	1.01	-3.16	-1.77	1.38
Na^+-$C_{24}H_{12}$-C	-32.95	-10.08	-4.69	5.39
Na-$C_{24}H_{12}$-E	-1.09	-3.28	-1.20	2.08
Na^+-$C_{24}H_{12}$-E	-33.44	-9.99	-4.67	5.32
Na-$C_{54}H_{18}$-C	-9.52	-3.59	-1.96	1.63
Na^+-$C_{54}H_{18}$-C	-37.12	-8.65	-4.36	4.29
Na-$C_{54}H_{18}$-I	-9.14	-3.57	-1.99	1.58
Na^+-$C_{54}H_{18}$-I	-37.16	-8.59	-4.35	4.24
Na-$C_{54}H_{18}$-E	-9.84	-3.63	-1.93	1.71
Na^+-$C_{54}H_{18}$-E	-37.19	-8.46	-4.35	4.11

3. RESULTS AND DISCUSSION

3.1 Adsorption on Graphene Quantum Dots

All geometry optimizations in this study were carried out using the M06-2X/6-31G+(d) level of theory, as shown in Figure 2. The choice of the M06-2X functional, which incorporates dispersion correction, is based on its proven efficacy in accurately predicting non-covalent interactions, as indicated by previous studies (Kuamit et al., 2025; Mulya et al., 2024; Mulya and Parasuk, 2020). This function is particularly suited for studies involving weak interactions, such as those between a sodium atom or ion and the graphene quantum dots (GQDs) model. The incorporation of dispersion corrections is crucial for obtaining reliable results in systems where van der Waals forces play a significant role.

As shown in Table 1, the adsorption energy of a sodium atom or ion on coronene and circumcoronene GQDs was systematically investigated using Equation 1 to understand their interaction dynamics and potential implications for sodium-ion battery performance. This investigation has provided significant insights, particularly regarding the interaction dynamics and their relevance to sodium-ion battery technologies. Here, we delve deeper into the adsorption energies and the effects of sodium atom and ion adsorption on these GQDs.

In coronene, the adsorption process exhibits distinct preferences depending on the adsorption sites and the nature of the sodium species (atom vs. ion). Sodium atom at the central site of coronene GQDs showed a relatively weak adsorption energy of 1.01 kcal/mol, indicating that this interaction is unstable adsorption (Mulya et al., 2024) and might require external forces for stabilization. However, the edge sites demonstrated a stronger, physisorptive interaction with a notably negative adsorption energy of -1.09 kcal/mol. This suggests that the edge sites, with their higher π-electron density and availability of reactive sites, facilitate a more spontaneous and energetically favorable adsorption. Sodium ion, on the other hand, showed significantly higher adsorption energies across both sites: -32.95 kcal/mol at the center and -33.44 kcal/mol at the edge. This stark contrast in adsorption energies between neutral atom and ion can be attributed to the strong electrostatic forces between the positively charged sodium ion and the negatively charged electron clouds of the GQDs. The slightly higher adsorption energy at the edge for ion also underscores the enhanced electrostatic and chemical interactions possible at these sites.

Moving to circumcoronene, the adsorption energies, while more uniformly distributed, still highlighted a preference for the edge sites. The edge sites registered the most negative adsorption energy at -9.84 kcal/mol compared to -9.52 kcal/mol at the center and -9.14 kcal/mol at the intermediate sites. This pattern suggests that, similar to coronene, the edge sites in circumcoronene are more chemically active and capable of stronger interactions with sodium atom. For sodium ion, the adsorption energies were closely packed but still slightly more negative at the edge (-37.19 kcal/mol) compared to the center (-37.12 kcal/mol) and intermediate (-37.16 kcal/mol). These results indicate that like in coronene, the edge sites in circumcoronene provide a more favorable environment for ion adsorption due to enhanced electrostatic and chemical interactions.

The comparison between the adsorption behaviors on coronene and circumcoronene GQDs reveals that while both types of GQDs preferentially adsorb sodium at the edges, circumcoronene exhibits slightly higher overall adsorption energies for both atom and ion. This could be due to the larger size of circumcoronene, which may offer more extensive reactive surfaces and potentially more favorable electronic environments

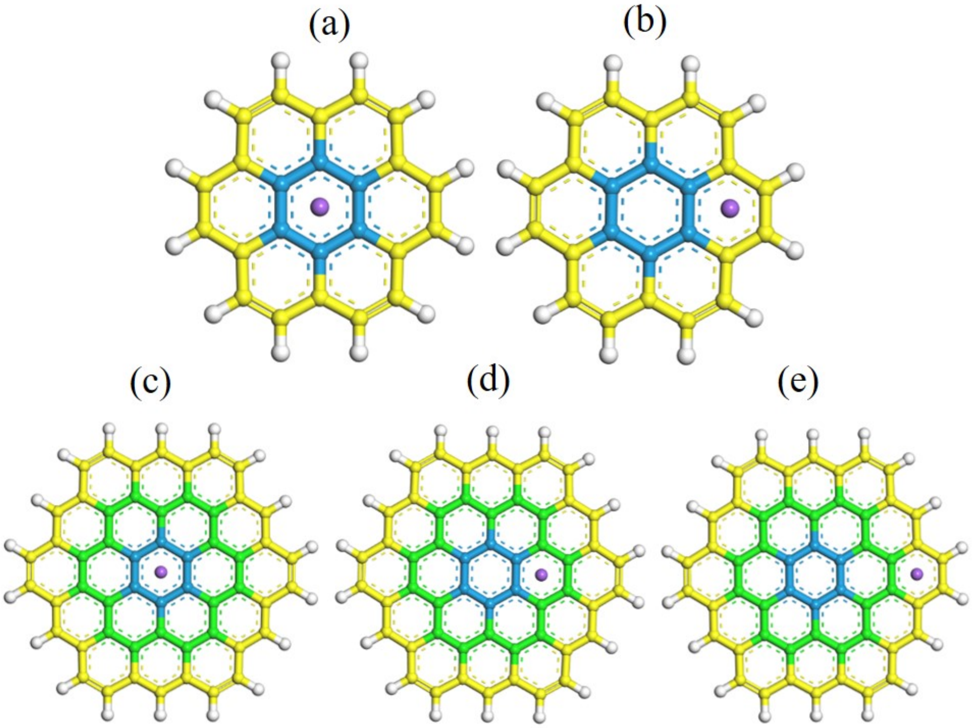

Figure 2. Geometry Optimization of: (a, b) Central and Edge Locations of Coronene; (c, d, e) Central, Intermediate, and Edge Locations of Circumcoronene

for interaction.

Comparing our study with Pattarapongdilok and Parasuk (2020), both highlight the critical role of GQD edge sites in enhancing alkali metal ion interactions, crucial for battery applications. In both studies, sodium and lithium atom show a preference for edge sites due to lower adsorption energies, with ion exhibiting stronger binding due to electrostatic interactions. Our research found sodium ion with adsorption energies of -32.95 kcal/mol at the center and -33.44 kcal/mol at the edge, while Pattarapongdilok and Parasuk (2020) reported even stronger lithium ion interactions, particularly with negatively charged GQDs, exceeding 100 kcal/mol. This difference is attributed to lithium's smaller ionic radius and higher charge density, resulting in stronger binding compared to sodium. Both studies demonstrate a size-dependent adsorption energy trend, with larger GQDs providing more reactive surfaces, yet consistently favoring edge sites across different GQD sizes and types.

These insights are crucial for optimizing GQD-based anode materials in sodium and lithium-ion batteries, aiding in the design of more efficient and sustainable energy storage systems. Understanding these adsorption dynamics is essential for enhancing the storage capacity, stability, and overall performance of sodium-ion batteries, contributing to the development of advanced battery technologies aligned with global efforts to combat climate change.

3.2 Effect of Sodium Adsorption on The Energy Gap

The relationship between sodium adsorption and the energy gap in graphene quantum dots (GQDs) derived from coronene and circumcoronene are crucial for their application in sodium-ion batteries. This relationship significantly affects the electrical conductivity of GQDs, influencing battery performance during charging and discharging cycles. The energy gap in semiconductor materials indicates how easily electrons can move from the valence band to the conduction band. A smaller energy gap generally corresponds to higher electrical conductivity, which is desirable in battery electrodes for efficient charge transport. To measure the energy gap, we can follow Equation 2.

In our study, sodium adsorption impacts the energy gap dynamics of GQDs, revealing distinct behaviors in coronene and circumcoronene structures under different conditions. As shown in Table 1 and Figure 3, the adsorption of both a sodium atom and a sodium ion reduce the energy gap of GQDs derived from both coronene and circumcoronene.

For coronene GQDs, sodium atom, simulating the discharging condition, causes a notable reduction in the energy gap. Specifically, at the central site, the gap decreases from 5.84 eV to 1.38 eV. This significant reduction enhances the GQD's conductivity, facilitating efficient electron transfer during discharging. Conversely, sodium ion, representing the charging condition, lead to a less pronounced reduction in the energy gap, from 5.84 eV to 5.39 eV at the central site. This

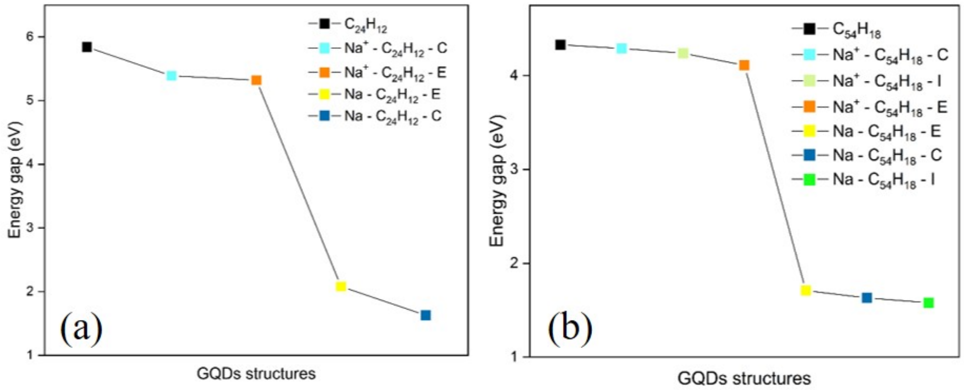

Figure 3. Energy Gaps of Un-Adsorbed and Na/Na$^+$ Adsorbed on (a) Coronene and (b) Circumcoronene GQDs

modest decrease suggests a lesser enhancement in conductivity, potentially impacting charging efficiency and speed.

Similarly, for circumcoronene GQDs, sodium atom effectively reduces the energy gap across various adsorption sites, such as decreasing from 4.33 eV to 1.63 eV at the central site. This reduction improves conductivity and enhances the material's semiconductor properties during discharging. Sodium ion, however, result in a lesser reduction in the energy gap, lowering it to 4.29 eV at the central site, indicating only a modest increase in conductivity, which might not significantly benefit charging compared to the substantial improvements observed during discharging with sodium atom.

These findings underscore the critical role of sodium adsorption in modulating the electronic properties of GQDs, influencing their potential in sodium-ion batteries. This trend aligns with previous study Hosseinian et al. (2017) reported that both sodium atom and ion adsorption can reduce the energy gap in anode materials, using graphene, SiC, BN, and AlN nanosheets in Na−ion batteries. The differential impact of sodium atom and ion on the energy gap and, consequently, on the conductivity of GQDs has significant implications for battery performance. During discharging (sodium atom), the large decrease in the energy gap ensures high conductivity, facilitating rapid and efficient electron flow. During charging (sodium ion), the smaller reduction in the energy gap results in less enhanced conductivity, potentially leading to slower charging times and less efficient energy storage. This phenomenon is consistent across both central and edge adsorption sites, though the magnitude of change varies. Typically, the central sites show a more pronounced effect, possibly due to more symmetric interaction and effective overlap of electronic states at these locations.

Understanding the distinct effects of sodium atom and ion adsorption on the energy gaps of coronene and circumcoronene GQDs is crucial for optimizing these materials for sodium-ion battery applications. The insights gained can guide the design of GQD-based anodes that optimize performance across both charging and discharging cycles, enhancing overall battery efficiency and sustainability. This knowledge also contributes to the broader field of materials science, where electronic property manipulation through adsorbate interactions plays a critical role in developing advanced functional materials.

3.3 Application of Graphene Quantum Dots in Sodium-Ion Batteries (SIBs)

Graphene Quantum Dots (GQDs), derived from materials like coronene and circumcoronene, present a promising frontier for anodes in sodium-ion batteries (SIBs). Their unique electronic and structural properties offer potential improvements over traditional anode materials. This section discusses the theoretical voltage and specific electrochemical reactions, as reported by previous study (Hosseinian et al., 2017; Louis et al., 2023; Nejati et al., 2017), the electrochemical reactions at the anode and cathode are described as follows:

- Anode Reaction :

$$Na/GQDs \rightleftharpoons Na^+/GQDs + e^- \tag{3}$$

This reaction involves the oxidation of sodium adsorbed on the GQD, releasing an electron and forming sodium ion.

- Cathode Reaction

$$Na^+ + e^- \rightleftharpoons Na \tag{4}$$

- Overall Cell Reaction

$$Na^+ + Na/GQDs \rightleftharpoons Na^+/GQDs + Na + \Delta G_{sel} \tag{5}$$

This reaction represents the total electrochemical process occurring within the cell, involving both the anode and cathode reactions.To determine the cell voltage (V_{sel}), we apply the Nernst equation as follows:

$$V_{sel} = \frac{-\Delta G_{sel}}{zF} \tag{6}$$

where z is the charge of the sodium ion Na^+ and F is the Faraday constant (96.500 C mol^{-1}). ΔG_{sel} represents the change in Gibbs free energy for the overall cell reaction.

Table 2. Theoretical Voltage (V) of Sodium Adsorption on Coronene and Circumcoronene

GQDs	Central	Intermediate	Edge
$C_{24}H_{12}$	1.47	-	1.40
$C_{54}H_{18}$	1.20	1.22	1.19

Following Equations 3 to 6, we present the theoretical voltage of sodium-ion batteries with coronene- and circum-coronene-based GQD anodes, as shown in Table 2. For batteries employing coronene-based GQDs as anodes, the theoretical voltage at the central adsorption site is higher (1.47 V) compared to the edge site (1.40 V). This variation underscores the influence of the adsorption site on electrochemical properties. In contrast, circumcoronene GQDs exhibit the highest theoretical voltage of 1.22 V when sodium is adsorbed at the intermediate site, with slightly lower voltages at the central (1.20 V) and edge (1.19 V) sites. Despite being marginally lower than those of coronene, circumcoronene remains a viable candidate for sodium-ion battery applications, particularly considering its structural stability and material availability. A comparison of adsorption sites-central, intermediate, and edge-is shown in Figure 4.

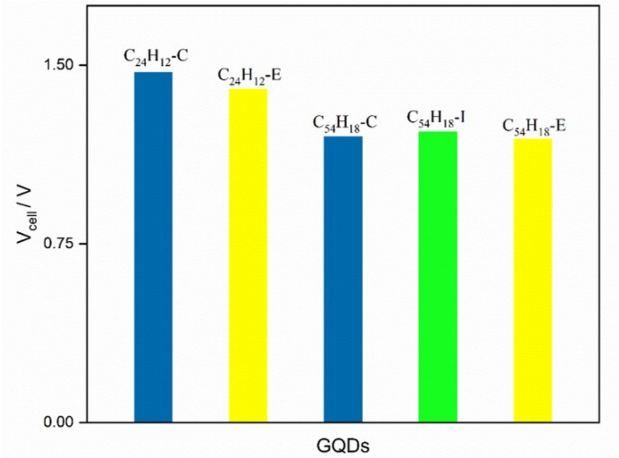

Figure 4. The Cell Voltage of Different Graphene Quantum Dots (Gqds) is Used as Anodes in Sodium-Ion Batteries: Central Area (Blue), Intermediate Area (Green) and Edge Area (Yellow)

When compared to previous studies on aluminum-ion batteries (Mulya and Parasuk, 2020), which reported theoretical voltages ranging from 4.24 to 4.33 V for coronene and 3.86 to 3.95 V for circumcoronene, the sodium-ion battery voltages are lower. This difference is primarily due to the different ion interactions and adsorption energies. Aluminum-ion batteries benefit from stronger adsorption energies, resulting in higher voltages. However, the lower voltage in sodium-ion batteries is balanced by other advantages such as availability and stability of materials.

Table 3. Comparison of GQD Anode Materials with Other Anode Materials for Sodium-Ion Batteries Based on Energy Adsorption (E_{ads}), Energy Gap (E_g) in Ev, and Theoretical Voltage (V_{cell}) in Volts

Materials	E_{Ads}	E_g	V_{cell}	References
$C_{24}H_{12}$-GQDs	-1.09	2.08	1.40	Our work
$C_{54}H_{18}$-GQDs	-9.84	1.71	1.22	Our work
AlN nanosheets	-3.70	0.96	1.49	(Hosseinian et al., 2017)
BN nanosheets	-0.10	1.64	1.46	(Hosseinian et al., 2017)
Graphene	-22.20	0.29	0.65	(Hosseinian et al., 2017)
SiC nanosheets	-27.70	0.12	0.61	(Hosseinian et al., 2017)

Comparing our results with other anode materials for sodium-ion batteries, as shown in Table 3, we demonstrate the competitive performance of GQDs in terms of adsorption energy, energy gap, and cell voltage. Although coronene-based GQDs exhibit a moderate adsorption energy of -1.09 eV and a cell voltage of 1.40 V, their small size limits their effectiveness compared to circumcoronene-based GQDs. Circumcoronene GQDs show stronger adsorption energy (-9.84 eV), suggesting better stability than AlN (-3.70 eV) and BN nanosheets (-0.10 eV), though less than graphene (-22.20 eV) and SiC (-27.70 eV). However, the excessively strong adsorption in graphene and SiC might hinder ion mobility. The moderate energy gap of circumcoronene GQDs (1.71 eV) ensures a balance between conductivity and stability, unlike the very small gaps in graphene (0.29 eV) and SiC (0.12 eV), which may lead to less control over side reactions. While the cell voltage of circumcoronene GQDs is competitive at 1.22 V, AlN and BN nanosheets offer slightly higher voltages of 1.49 V and 1.46 V, respectively. Overall, Table 3 provides a clear comparison, underscoring the efficiency of our materials relative to existing candidates. This comprehensive evaluation highlights the importance of considering a holistic view of material properties, including theoretical voltage, stability, and availability, when selecting optimal materials for advanced battery technologies. Such comparisons are crucial for guiding future research and development in the field of sodium-ion batteries.

4. CONCLUSIONS

This study demonstrates the potential of coronene and circumcoronene-based graphene quantum dots (GQDs) as promising anode materials for sodium-ion batteries (SIBs). Through theoretical voltage calculations, adsorption energy analysis, and examination of sodium adsorption impacts on the energy gap, we have shown that these GQDs can enhance the electrochemical performance of SIBs. Specifically, coronene GQDs exhibit higher theoretical voltages of up to 1.47 V and significant reductions in the energy gap from 5.84 eV to 1.38 eV, indicating enhanced conductivity. Circumcoronene GQDs, while slightly lower in voltage at 1.22 V, still offer considerable improvements with energy gap reductions from 4.33 eV to 1.63 eV. These findings suggest that coronene GQDs, with their higher theoretical voltages, offer significant improvements over traditional materials, while circumcoronene GQDs provide viable alternatives due to their stability and availability. This research advances the field by addressing key limitations in SIB technology, paving the way for more efficient, sustainable, and cost-effective energy storage solutions.

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