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Templating nanostructured aromatic based materials as possible anode electrodes for Na-ion batteries: A computational DFT approach

A. Ahmad [1], A.A.M.Abahussain [2], M.H.Nazir [3], S.Z.J. Zaidi [1,4]*

[1] Institute of Chemical Engineering and Technology, University of the Punjab, Pakistan.
[2] Department of Chemical Engineering, College of Engineering, King Saud University, Riyadh 11421, Saudi Arabia
[3] Faculty of Computing Engineering and Sciences, University of South Wales, United Kingdom.
[4] Laboratory for Energy Water and Healthcare Technologies, University of the Punjab, Pakistan.

Corresponding Author Email: zohaib.icet@pu.edu.pk

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ABSTRACT

Due to their widespread availability and lower costs Na-ion batteries have grabbed attention as a promising substitute for lithium-ion batteries. In this paper, we delve into a computational investigation of the potential use of 2,4-Chloronitrotoluene and pyrazine as electrode materials for SIBs. We utilized Density Functional Theory (DFT) calculations to examine their properties and suitability for energy storage applications. Adsorption energies, highest occupied molecular orbital, lowest unoccupied molecular orbital, HLG energies, total energies, and bond lengths were computed using computational theories for aromatic compounds. This computation is based here on the DFT and computational engineering modelling approach. The results indicate that both 2,4-chloronitrotoluene and pyrazine exhibit favorable adsorption energies for Na-ion adsorption, indicating their potential as electrode materials. Furthermore, the investigation delved into the electronic properties of the materials. Notably, the analysis showed that the E_{HOMO}, E_{LUMO}, and E_{HLG} are facilitative to the efficient transfer of electrons during the operation of the battery. Moreover, the computed bond lengths indicate that stable Na-ion adsorption can appear on both materials, further solidifying their potential for integration into the framework of Na-ion batteries. In essence, this study yields valuable insights into the electrochemical aspects of 2,4-chloronitrotoluene and pyrazine, highlighting their promising candidacy as electrode materials for SIBs.

NOMENCLATURE

CN	2,4-chloronitrotoluene
PR	Pyrazine
DFT	Density functional theory
SIBs	Sodium ion batteries
HOMO	Highest occupied molecular orbital
LUMO	Lowest unoccupied molecular orbital
HLG	HOMO LUMO Gap
B3LYP	Becke, 3-parameter, Lee–Yang–Parr

Subscripts

ad	adsorption
homo	highest occupied molecular
lumo	lowest unoccupied molecular orbital

1. INTRODUCTION

Na-ion batteries have garnered significant attention as a favorable substitute to the prevalent Li-ion batteries, which presently dominate the storing energy landscape. Sodium, being more abundant and cost-effective than lithium, presents a sustainable choice for storing energy on large scale, marking a important step towards a more sustainable environment [1]. Sodium-ion batteries present hope for a greener future. By using sodium ions rather of the more common lithium ions, these batteries are not only cheaper but also better for the environment [2].

A key advantage of sodium-ion batteries lies in their utilization of abundant materials. With sodium ranking as the sixth most abundant element on our planet, its general availability exceeds that of lithium. This intrinsic abundance implies that scaling up the production of sodium-ion batteries could be achieved more seamlessly, without facing the geopolitical challenges associated with lithium-ion battery production [3]. Moreover, the materials used in sodium-ion batteries are generally safer and less harmful than those used in lithium-ion batteries. LIBs often lean on resources like cobalt, which are frequently sourced under environmentally damaging and ethically concerning conditions [4]. Contrariwise, sodium-ion batteries can utilize materials like Mg, which are more abundant and environmentally sustainable. This distinction positions sodium-ion batteries as potentially more cost-effective than their lithium-ion counterparts [5]. With the surge in battery demand, the limitations and increasing prices of lithium are becoming evident. In contrast, the vast availability and affordability of sodium present a more sustainable avenue for large-scale battery production [6]. Furthermore, sodium-ion batteries have the potential to offer higher energy densities and more extended lifetimes when compared to LIBs. However, making high-performance SIBs comes with its own set of challenges, such as dealing with the relatively larger size of Na ions and the absence of appropriate electrode materials [7].

Sodium-ion batteries (SIBs) function based on the same basic principle as other rechargeable batteries, involving the movement of ions between two electrodes through an electrolyte during charging and discharging cycles. In the case of SIBs, the charge carriers are sodium ions (Na+), in contrast to lithium ions used in lithium-ion batteries [8]. During the charging process, sodium ions are drawn from the cathode material, generally made of layered transition metal oxides or polyanionic compounds. These ions cross through the electrolyte, usually a salt dissolved in an organic solvent, and get stored in the anode material, generally composed of carbon. Meanwhile, electrons transfer through the external circuit to the anode, creating a voltage difference between the two electrodes [9]. When the battery discharges, the process inverts. The stored Na ions in the anode travel back to the cathode through the electrolyte, while electrons float in external circuit, generating an electric current to power devices. This cycle can be replicated multiple times, enabling the battery to be recharged and used again [10].

The performance SIBs relies on various factors, including the choice of electrode and electrolyte materials, the structure of the cell, and the operating conditions. One of the primary challenges in SIB development is the quest for materials that can present high capacity, stable cycling, and fast charge/discharge rates while being cost-effective and abundant. Some studies have also concentrated on transition metal oxides for various electrochemical aspects of energy generation and storage [11]. Continued research in this domain seeks to enhance the efficiency and reliability of SIBs for diverse energy storage applications. 2,4-Chloronitrotoluenes and pyrazine have appeared as promising anode materials for Na-ion Batteries (SIBs) due to their strong conductivity and capacity. 2,4-Chloronitrotoluenes, a type of carbon with a special cylindrical structure, offer a considerable surface area and superior electrical conductivity [12]. On the other hand, pyrazine is an organic molecule with a flat structure that can host sodium ions between its layers [13]. This study employed density functional theory (DFT) to examine 2,4-chloronitrotoluenes and pyrazine, providing valuable insights into their electrochemical properties as anode materials for SIBs. These understandings have played a pivotal role in driving the design and enhancement of these materials to boost battery performance. Key properties such as adsorption energies, HOMO energy, LUMO energy, and the energy difference between HOMO and LUMO orbitals were closely examined.

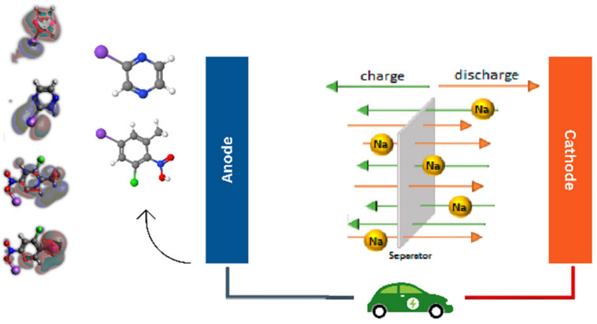

Figure 1: New Sodium-Ion Battery Materials: 2,4-Chloronitrotoluene and Pyrazine

2. COMPUTATIONAL DETAILS

Our research methodology relied on an ab initio approach, using DFT calculations through computational engineering modeling package along with a molecular editor and visualizer [14,15]. The main aim of our research was to gain insights into the fundamental electronic properties of electrode materials. We specifically concentrated on analyzing a single atomic layer of these materials. To achieve this, we examined adsorption energies, E_{HOMO}, E_{LUMO}, and E_{HLG}, considering the geometrically optimized structures using density functional theory (DFT). We adjusted the vibrational frequencies to guarantee that the calculated geometries accurately represented the local minimum points [16]. The structures of 2,4-chloronitrotoluenes and Pyrazine with Sodium ion were constructed using the DFT/B3LYP approach. For various tasks such as structure optimization and energy calculations, the method selected was ground state, utilizing DFT with default spin, and the Basis was selected as 6-31G.

3. RESULTS AND DISCUSSIONS

3.1 Geometrically optimized structures of 2,4-Chloronitrotoluenes and Pyrazine with Na

This study involved an analysis of the interaction between sodium ions and 2,4-Chloronitrotoluenes and Pyrazine molecules. The investigation entailed an examination of four distinct optimized structures for each compound. Optimized structures were generated by systematically altering the positions of sodium ions within the molecular framework. The optimization was conducted using the 'optimization' job type, and DFT served as the ground-state method. The calculations were performed with default spin settings and a 6-31G basis set, providing insights into the most energetically favorable configurations of sodium ions within the molecules. The results obtained from this study have meaningful implications for the potential use of these molecules as electrode materials in SIBs.

In Figure 2, we showcase a visual representation of our optimized structures of 2,4-chloronitrotoluene with sodium ion configurations, providing insight into their spatial arrangement and geometry.

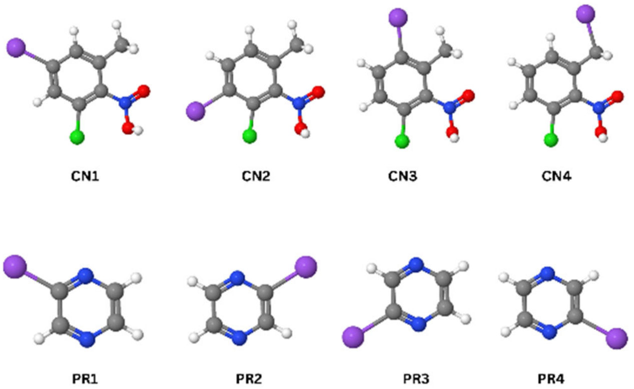

Figure 2: Optimized Structures of 2,4-Chloronitrotoluenes and Pyrazine with Sodium Ions

3.2 Theoretical capacity and Energy density

The Theoretical capacity (**$Q_{theoretical}$**) of the battery can be calculated using Faraday's law:

$$Q_{theoretical} = C = nF / M \qquad (1)$$

The theoretical capacity, represented as **$Q_{theoretical}$**, is measured in Ah/g or Ah/cm³. Here, '**n**' represents the number of electrons participating in the redox reaction, '**F**' is the Faraday constant (96,485 C/mol), and '**M**' represents the molar mass of the active material. Pyrazine, having a molecular weight of 80.10 g/mol, is capable of engaging in a sodium-ion battery configuration with a distinct charge transfer reaction.

$$C_4H_4N_2 + Na^+ + e^- \rightarrow NaC_4H_4N_2 \qquad (2)$$

In this reaction, one electron is transferred per sodium ion, so n = 1. Plugging in the values, we get Q = 1204 Ah/g. The charge transfer mechanism for 2,4-CNT in a sodium ion battery is:

$$2,4\text{-}CN + Na^+ + e^- \rightarrow Sodium\ 2,4\text{-}CN \qquad (3)$$

In this reaction, one electron is transferred per sodium ion, so n = 1. The molar mass of 2,4-CNT is 181.59 g/mol. Plugging in the values, we get: Q = (1 x 96,485 C/mol) / 181.59 g/mol = 531 Ah/g.

In order to convert the units of theoretical Capacity from Ah/g to Wh/kg we need to multiply it with Vcell and divide it by 1000. In order to calculate Vcell we use $V_{cell} = \Delta G/nF$, Where F is Faradays constant n is charge on sodium Delta G is gibbs free energy. We used B3LYP 6-31+G basis for calculations. The values of V_{cell} of 2,4-Chloronitrotoluenes and pyrazine were calculated as 5.621 volts and 1.778 volts respectively and the energy densities are calculated as 2.991 Wh/kg and 2.140 Wh/kg respectively.

3.3 Sodium Ion Adsorption Energies

The adsorption energy of sodium in 2,4-Chloronitrotoluenes and pyrazine plays a crucial role in determining capacity of Na-ion intercalation, stability and durability of the anode material [18]. A high adsorption energy of sodium in 2,4-Chloronitrotoluenes and pyrazine can result in strong binding between the sodium ions and the electrode, which can improve rate capability and cycling stability of the electrode material. However, if the adsorption energy is too high, the sodium ions may become strongly trapped in the electrode material, which can reduce the capacity and voltage of the battery. [18] In our study we calculated the adsorption energies of sodium on different transition structures of 2,4-Chloronitrotoluene and Pyrazine by selecting the job as frequency and the method as ground state, DFT, default spin and the Basis as 6-31G in computational engineering modeling package. The adsorption energies can be calculated as [19].

$$E_{ad} = E_{total}(opt) - (E_{mon1}(opt) + E_{mon2}(opt)) \qquad (4)$$

Table 1: Adsorption Energies of Na ion on 2,4-CN

Transition State	E_{ad} (eV)
PR1	16.526
PR2	16.526
PR3	16.526
PR4	16.526

Table 2: Adsorption Energies of Na ion on Pyrazine

Tansition State	Bond Length (Å)
CN1	2.170
CN2	2.170
CN3	2.170
CN4	2.170

It can be seen from the above result that the adsorption energies of sodium in 2,4- Chloronitrotoluene varies between 21.621 eV to 30.068 eV the higher E_{ad} value for CN4 is due to the presence of a new lone pair on the 2,4-Chloronitrotoluene molecule. When a sodium ion adsorbs onto the 2,4-Chloronitrotoluene molecule, it can interact with the electron density in the molecule, including any lone pairs. The adsorption energy of sodium in Pyrazine was measured as 16.5266 eV. With respect to adsorption energy pyrazine is favorable electrode material because its adsorption energy is not too high like 2,4-Chloronitrotoluene. Sodium ions may become strongly trapped in the 2,4- Chloronitrotoluene, which can reduce the capacity and voltage of the battery.

3.4 Bond Lengths

The bond length between Na with 2,4-Chloronitrotoluene and pyrazine can have a significant effect on the working of a sodium-ion battery. In general, the shorter the length of bond between Na and anode material, the stronger the connection between them, which can improve the battery performance [20].

This happens due to sodium (Na) creating a strong connection with the anode material, it stores and carries Na ions within the material, boosting the battery's capacity and long-term stability. On the flip side, if the bond between them is too tight, it can restrict the movement of Na ions, leading to slow ion diffusion and ultimately reducing the battery's performance [21]. In our research we calculated the bond length of different transition states of Na with 2,4-Chloronitrotoluene and pyrazine. The results are expressed below.

Table 3: Evaluated bond length of different transition states

Transition State	Bond Length Å
PR1	2.170
PR2	2.170
PR3	2.170
PR4	2.170

of sodium with 2,4-Chloronitrotoluene

Table 4: Evaluated bond length of different transition states of sodium with Pyrazine

Transition State	E_{HOMO} (eV)	E_{LUMO} (eV)	E_{HLG} (eV)	E_{Total} (eV)
CN1	-5.596	-4.330	-1.266	-29866.473
CN2	-5.612	-4.368	-1.245	-29867.159
CN3	-5.583	-4.368	-1.215	-29859.199
CN4	-6.297	-4.543	-1.753	-29858.026

There was no difference observed between the bond lengths of Na with 2,4- chloronitrotoluene and pyrazine because in both cases the bond is between hydrogen and sodium.

3.5 Molecular Orbital Energies

The performance of SIBs can be significantly affected by the energy levels of the molecular orbitals in the anode materials. In the context of an SIB, the active electrode material undergoes a reversible process of inserting and removing Na ions during the charge and discharge cycles. This entire mechanism is dictated by the disparity in energy between the molecular orbitals of the electrode material and the Na ions [22]. More specifically, the energy level of the highest occupied molecular orbital (HOMO) of the electrode material affects the ease of Na ion insertion, while the energy level of the lowest unoccupied molecular orbital (LUMO) impacts the ease of Na ion removal [23]. If the energy level of the HOMO is too high, it can hinder the insertion of Na ions into the electrode material, leading to lower capacity and slower rate capability. Conversely, if the energy level of the LUMO is too low, it can make it difficult for the Na ions to de-insert, resulting in poor cycling stability [24].

In our study, we performed calculations to determine the energy levels of HOMO (Ehomo) and LUMO (Elumo), as well as the energy difference between them, for four different optimized structures of 2,4-Chloronitrotoluene and pyrazine. Figures 3 and 4 visually depict charge transfer processes in these molecules interacting with sodium ions, highlighting the roles of HOMO and LUMO orbitals in understanding electronic structure and energy levels. Additionally, we computed the total energy of the complex formed by the Na ions interacting with the electrode material. The total energy refers to the overall energy associated with the entire system, which includes both the electrode material and the Na ions. It represents the thermodynamic stability of the system and is a fundamental quantity in computational chemistry.

Table 5: Energy of HOMO, energy of LUMO, difference energy between HOMO and LUMO and total Energy of Na on 2,4-Chloronitrotoluene

Transition State	E_{ad} (eV)
CN1	21.621
CN2	20.935
CN3	20.935
CN4	30.068

Table 6: Energy of HOMO, energy of LUMO, difference energy between HOMO and LUMO and total Energy of Na on Pyrazine

Transition State	E_{HOMO} (eV)	E_{LUMO} (eV)	E_{HLG} (eV)	E_{Total} (eV)
PR1	-8.360	-5.311	-3.049	-11589.365
PR2	-8.115	-5.356	-2.759	-11589.365
PR3	-8.361	-5.311	-3.049	-11589.36495
PR4	-8.361	-5.311	-3.049	-11589.365

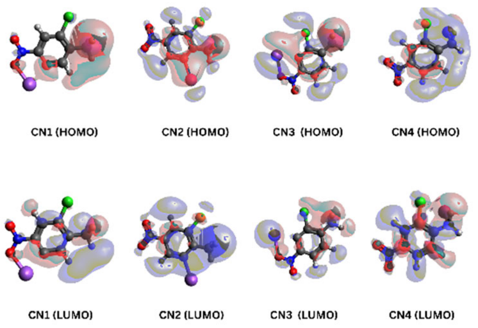

Figure 3: HOMO and LUMO Orbitals of 2,4-Chloronitrotoluene with Sodium Ions.

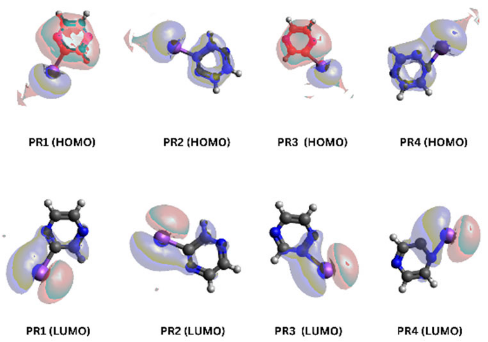

Figure 4: HOMO and LUMO Orbitals of Pyrazine with Sodium Ions.

As shown from the results that the **E_{HLG}** of 2,4-Chloronitrotoluene with sodium varies from -1.215 eV to -1.753 eV and for pyrazine with sodium it varies from -2.759 eV to -3.049 eV. So, 2,4-Chloronitrotoluene will be favorable because its **E_{HLG}** is not too high unlike pyrazine. In case of pyrazine when **E_{HLG}** is too high because of this the electrodes can lead to a higher risk of unwanted side reactions, such as electrolyte decomposition, which can degrade the battery's performance over time.

Table 7: Specific Capacitance, Energy density and Adsorption Energy of anode material for sodium ion batteries

Anode Material	**Specific Capacitance (F/g)**	**Enery Density (Wh/kg)**	**E_{ad} (eV)**	**Reference**
CNT loaded MnO2	140	21	-1.83	[25]
LiMn2O4	137	56	N.A	[26]
MnO2	45	43	3.77	[27]
Pyrazine	N.A	2.1	16.52	This Study
Activated Carbon	180	3.6	N.A	[27]
2,4-Chloronitro toluene	N.A	3	20.93	This Study

4 CONCLUSIONS

The research highlights the possibility of Na-ion batteries (SIBs) as a viable substitute to Li-ion batteries, citing the abundant and cost-effective nature of Na. Investigating 2,4-chloronitrotoluene and pyrazine as anode materials, the study emphasizes the influential role of sodium's adsorption energy, varying from 21.62 eV to 30.07 eV in 2,4-Chloronitrotoluene and 16.53 eV in pyrazine. Additionally, insights into E_{HOMO}, E_{LUMO}, and E_{HLG} provide valuable guidance for material optimization, improving energy density and overall SIB performance. This research signifies a notable step forward in the development of efficient and reliable SIBs for diverse applications of energy storage, paving the way for further improvements in the field.

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