

## Research Article

# A Theoretical Evaluation of the Energy and Power Density of Nickel Hydroxide for Hybrid Supercapacitor Applications

S.E Umoru<sup>1</sup> 

<sup>1</sup>Dept. of Physics, Federal University of Petroleum Resources, Effurun, Delta State, Nigeria

\*Corresponding Author: efemenaumoru@gmail.com

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**Abstract**— Achieving high energy density has remains a significant challenge in the development of supercapacitors. Supercapacitors that are hybrid, which incorporate the advantages of supercapacitors and batteries, have emerged a viable way to overcome the energy density restriction. The functionality of hybrid supercapacitor is built upon the type of materials that were utilized in its terminals. As a result, attention has been drawn to exploring various materials that can increase the energy performance of hybrid supercapacitor. This study has employed a theoretical approach, first principle calculation to calculate the parameters needed to evaluate the energy and power density of nickel hydroxide in order to assess its performance in hybrid supercapacitors. Base on the calculations, The power density, specific capacitance, and energy density were found to be  $1334.35\text{Fg}^{-1}$ ,  $450.89\text{Whkg}^{-1}$  and  $240.06\text{Wkg}^{-1}$  respectively. These results are well compared with the experimental results and have shown the viability of nickel hydroxide in hybrid supercapacitors.

**Keywords**— Density functional Theory, Energy density, Evaluation, First principle, Hybrid supercapacitors, Nickel hydroxide, Performance, Power density.

## 1. Introduction

The need for high-performance devices used for storing energy has grown exponentially in recent year due to the increasing need for compact electronic devices, electric vehicles, and renewable energy systems. Among energy storage, supercapacitors have emerged as promising candidates for efficient energy storage, providing an outstanding density of power, long cycle life, and rapid rates of charge and discharge [1,2]. But reaching an excessive energy density remains a significant challenge in the development of these devices. Supercapacitors with hybrid designs, which merge the advantages of both conventional supercapacitors and batteries, have emerged as a potential way out of the restrictions of energy density [3].

The performance of hybrid supercapacitor devices depends solely on the type of materials used in the fabrication of its electrodes [4]. As a result, researchers have turned their attention to exploring various materials that can increase the energy performance of hybrid supercapacitor technologies. One such material that has gained significant interest is nickel hydroxide  $\{\text{Ni}(\text{OH})_2\}$ . Nickel hydroxide is a good option for hybrid supercapacitors due to its unique electronic and structural properties [1]. Nickel hydroxide exhibits a layered crystal structure, where nickel ions are surrounded by hydroxide ions [5]. The layered structure of nickel hydroxide

allows for the intercalation and de-intercalation of ions, making it suitable electrode material for hybrid supercapacitors [6]

However, the full knowledge of nickel hydroxide electrode for hybrid supercapacitor has not been fully realized, basically as a result of limited or non availability of a comprehensive knowledge of its electronic and structural properties at the atomic level. Although several experimental studies have been conducted to investigate its performance in energy storage devices such as battery, their findings have often been limited by the complexity (such as multiple phases and transformations, structural defects and disorder) and variability of the material's structure. To overcome the limitations imposed by the complexity and variability of nickel hydroxide's structure, a theoretical approach such as first principle calculation can be employed to calculate the parameters needed to evaluate its performance when put to use in hybrid supercapacitors. First principle calculation involves utilizing estimation involving quantum mechanical to study the compulsory properties of compounds at the atomic level. These calculations can complement experimental studies by providing insights into the performance of nickel hydroxide under different conditions. First principle calculations utilize computational techniques such as density functional theory (DFT) to have knowledge of the atomic-level architecture, energy, and behavior of nickel hydroxide. This study has employed DFT to calculate the

parameters needed to evaluate its performance in hybrid supercapacitors. DFT allows for a more accurate and full explanation of the electronic architecture and energy of materials by considering the interactions between electrons and the atomic nuclei [7]. It takes into account the electrons and provides a more realistic representation of the material's properties [8]. Without the need for empirical data, DFT enables precise predictions of various properties such as energy level, electronic band properties, Density of state (DOS), reaction energy, and charge distribution [9].

This study aims to evaluate the performance of nickel hydroxides in hybrid supercapacitors by gaining insight into its electronic and structural properties such as valency, band gap, lattice parameter, inter-atomic distance in order to assess its stability and examine the charge density distribution within the material and explore its correlation with energy storage performance. This investigation provides an important promise for the creation of more efficient and sustainable energy storage devices, contributing to the advancement of renewable energy technologies and the transition to a greener future.

This research work is organized as follows; section 1 contains the introduction of the research work, section 2 gives details of work that has been done which are related to this work, section 3 contains theories and calculation that back up this research work, section 4 gives the details of the methodology applied that led to the results, section 5 provides the results and the explanation of the results, section 6 gives the conclusion and future scope of the work.

## 2. Related work

Supercapacitors are devices for storing energy that offer high power density and rapid charging potential. The development of supercapacitors for standalone energy storage applications was slowed down by their comparatively low energy density. In contrast, batteries are energy storage devices characterized by low power density but high energy density. In efforts to address the limitations faced by batteries and traditional supercapacitors, researchers have put forward the idea of hybrid supercapacitors. These hybrid supercapacitors present an opportunity to enhance the performance of both batteries and supercapacitors by merging the high power densities characteristic of supercapacitors with the superior energy densities of batteries. By utilizing advanced materials with enhanced attributes, hybrid supercapacitors are capable of achieving increased energy density while maintaining the rapid charging and discharging features of supercapacitors. In order to determine nickel hydroxide's superiority in hybrid supercapacitors, researchers have carried out a number of studies on the material. For example, Weili et al. (2022)[10] conducted a research work titled "Sulfate assisted synthesis of  $\alpha$ -type nickel hydroxide nanowires with 3D reticulation for energy storage in hybrid supercapacitors". This study investigates the creation of  $\alpha$ -type nickel hydroxide nanowires featuring a 3D reticulated structure for application in hybrid supercapacitors. The research emphasizes the impressive specific capacity and excellent cycling stability of these

nanowires. Due to its innovative 3D porous structure and  $\alpha$ -type phase configuration, the newly developed NSOH NW electrode achieves an impressive specific capacity of 246.3 mA h g<sup>-1</sup> at a current density of 1 A g<sup>-1</sup>, along with a remarkable cycling stability of 91.7% after 4000 cycles. Additionally, the assembled NSOH NWs//AC HSCs can deliver a high energy density of 59.8 W h kg<sup>-1</sup> while maintaining a power density of 830.3 W kg<sup>-1</sup>. The HSCs also exhibit a specific capacity retention of 91.5% after undergoing 10,000 cycles. These findings demonstrate that the proposed NSOH NWs, with their 3D network structure, hold considerable promise for advanced HSC applications. Jiang et al. (2015)[11] also reported a work titled Ternary hybrids of amorphous nickel hydroxide-carbon nanotube conducting polymer for supercapacitors with high energy density, excellent rate capability, and long cycle life. According to the authors, utilizing the ternary Ni(OH)<sub>2</sub> hybrid for the positive electrode and reduced graphene oxide/carbon nanotube hybrid for the negative electrode, the resulting asymmetric supercapacitors demonstrate a significant energy density of 58.5 W h kg<sup>-1</sup> at a power density of 780 W kg<sup>-1</sup>, along with an impressive cycle life (retaining 86% of capacitance after 30,000 cycles). The design of the ternary hybrid architecture for amorphous Ni(OH)<sub>2</sub> can be considered a general strategy to achieve pseudocapacitive materials for supercapacitors that provide both high energy density and excellent rate performance, in addition to long cycle longevity. Brisse et al. (2018) [12], in their research titled Ni(OH)<sub>2</sub> and NiO Based Composites: Battery Type Electrode Materials for Hybrid Supercapacitor Devices, explored the application of Nickel hydroxide as a battery-type electrode within hybrid supercapacitors. The authors indicated that at a scan rate of 1 mV·s<sup>-1</sup>, the capacity of the Ni(OH)<sub>2</sub> sintered electrode is 223 C·g<sup>-1</sup>, which constitutes 22% of its theoretical capacity.

### 2.1 Overview of Energy Storage Technology

Energy storage technologies are essential to our contemporary society because they let us to effectively store and use energy whenever it's really required. These technologies assist in closing the disparity amid the production and utilization of energy, making renewable energy sources more reliable and ensuring a stable and resilient grid. Among the most prominent energy storage solutions are batteries and supercapacitors. In this section, we will delve into the intricacies of hybrid supercapacitor technologies, exploring its working principles, applications, advantages, and limitations.

### 2.2 Hybrid supercapacitors-based energy storage technologies

Supercapacitors, often referred to as electrochemical capacitors or ultracapacitors, are devices for storing energy which employ electrostatic charge separation to store energy. They offer high power density and quick release of energy, making them appropriate for use in devices requiring quick bursts of energy [13]. Novel energy storage technologies called hybrid supercapacitors blend the immense power density of supercapacitors with the abundant energy of batteries. Technology in hybrid supercapacitors includes: Li-

ion hybrid supercapacitors (LIHSCs) and Battery-Supercapacitor Hybrid Energy Storage Systems (HESS) [14].

Li-ion hybrid supercapacitors (LIHSCs) are very sophisticated energy storage devices that combine supercapacitors' substantial power density with lithium-ion batteries' excellent energy density. With a special blend of quick charging and discharging speeds and significant energy storage, they are made to offer a compromise between the two technologies. LIHSCs use a carbon-based negative electrode material that is pre-doped with lithium ions to increase energy density [15]. This material is able to absorb lithium ions. Unlike conventional supercapacitors, the positive electrode functions using the Electrical Double Layer (EDL) principle, and the negative electrode experiences lithium redox processes similar to those in lithium-ion batteries [16]. LIHSCs are distinguished by their great safety, long life, and high power density [17]. They have a cycle life of over 100,000 cycles and can be charged and discharged at rates higher than 100C, which is much greater than lithium batteries' [18]. A single volume energy density of 10~15 Wh/L is possessed by LIHSCs, which have an energy density three to five times higher than that of conventional supercapacitors. The LIHSC's negative electrode is constructed from carbon compounds used in lithium-ion batteries, whereas the positive electrode is formed of activated carbon [16]. Lithium ions are made easier to travel between the electrodes by the electrolyte, which is a solution of lithium salt. To store electrochemical energy in the organic electrolyte by means of electrostatic force, the capacitor component needs to possess a high level of electrical conductivity. LIHSCs have a number of benefits over conventional lithium-ion batteries and supercapacitors, such as a longer lifespan, tolerance to high temperatures, safety because of their non-flammable and non-explosive materials, and a lower energy density but a higher output density. Applications for LIHSCs can be found in a wide range of industries, such as rail transit, energy-saving elevators, golf carts, AGVs, DC circuits, smart meters, medical/healthcare, manufacturing, data centers, trams, fuel cell vehicles, forklifts, construction machinery, railroad/subway, ships/logistics, electric vehicles, rail transit, and wind pitch systems [19]. It can therefore be concluded that Li-ion hybrid supercapacitors, which provide a balance between the power delivery of supercapacitors and the energy storage capacity of lithium-ion batteries, are a noteworthy development in energy storage technology. Liquid interface controllers (LIHSCs) have the potential to be a significant player in energy storage and management in the future due to their distinctive features and expanding application space.

The Battery-Hybrid Supercapacitor Energy Storage configuration is an innovative technology for storing energy which overcomes the drawbacks of both technologies by combining the advantages of batteries and supercapacitors (SCs) [20]. The goal of this hybridization is to increase the energy storage system's lifespan, efficiency, and overall performance. The HESS has a number of benefits, such as longer battery life, higher energy recovery efficiency, and less stress on the batteries, which results in longer battery life [21]. Applications for HESS technology can be found in a

number of industries, such as wave energy converters, renewable energy systems, electric vehicles, and standalone micro-grid systems [22]. As HESS continues to be developed and optimized, new applications and performance improvements are anticipated, including the creation of energy management systems and control strategies.

### 2.3 Energy Storage Mechanism of Hybrid supercapacitor

The principles of electrostatic capacitors with two layers (EDLCs), where electrostatic particle accumulation occurs around the electrode-electrolyte interface, and pseudocapacitors, which require that the ions inside the electrolyte travel through a high-speed reversible network involving electro-sorption, faradaic redox, or embedded processes on electrode surfaces, govern hybrid supercapacitor devices (HSPs). A redox reaction occurs at the battery electrode, while a non-faradaic mechanism forms at the capacitive electrode in opposition.. Combining a non-Faradaic and a Faradaic mechanism has the benefit of increasing capacitance without causing the limitations associated with component mergers [23]. There are two varieties of hybrid supercapacitors: symmetric and asymmetric, depending on the arrangement of the electrodes. A schematic illustration of hybrid supercapacitor made up of a carbon electrode and a lithium insertion electrode is displayed in Fig.1. Based on the equation 1, the particular capacitance of battery-type is inversely equivalent to the product of the molar mass (M) of the participating materials and the operating voltage change (V), and directly related to the number of charge (n).

$$C_1 = \frac{n \times F}{M \times \Delta V} \quad (1)$$

Where F represents the Faraday constant

On the capacitive type of electrode, the capacitance has a direct relationship with the surface area 'A' and in direct proportion to the layer thickness (d) as shown in equation 2

$$C_2 = \frac{\epsilon}{d} A \quad (2)$$

The effective capacitance can be calculated from equation 3

$$\frac{1}{C_{eff}} = \frac{1}{C_1} + \frac{1}{C_2} \quad (3)$$

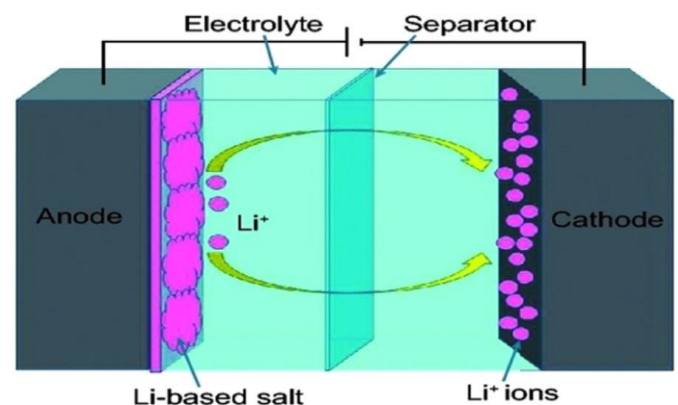


Figure. 1: Schematic illustration of a hybridized supercapacitor [24].

#### 2.3.1 Nickel Hydroxide-Based Hybrid Supercapacitors

Nickel hydroxide-based Hybrid supercapacitors merge the substantial power density of supercapacitors with the abundant energy density of nickel-based batteries. Utilizing

the advantages of both technologies, this hybridization aims to create a more efficient and versatile energy storage system. Nickel hydroxide, or  $\text{Ni}(\text{OH})_2$ , is widely used as the active element of the positive electrode in nickel-based hybrid supercapacitors [25]. Among its many amazing electrochemical qualities, its high specific capacitance and exceptional reversibility make it a suitable choice for energy storage applications [26]. In hybrid supercapacitors based on nickel hydroxide, pseudocapacitance is the main energy storage mechanism in the positive electrode. Through pseudocapacitance, which is determined by reversible redox mechanisms at the contact between the electrode and electrolyte, faradaic processes make it possible to store charge.

The negative electrode of hybrid supercapacitors based on nickel hydroxide is typically made of materials from carbon like activated carbon or carbon nanotubes. The carbon-based material provides a significant surface area for charge storage through the use of the electric double-layer capacitance (EDLC) mechanism.

In nickel hydroxide-based hybrid supercapacitors, an aqueous solution containing potassium hydroxide (KOH) or sodium hydroxide (NaOH) is frequently used as the electrolyte. The choice of electrolyte has an impact on the ionic conductivity and overall performance of the device. Hybrid supercapacitors hold a greater density of energy than normal supercapacitors because nickel hydroxide is used as the positive electrode material.

Their greater density of energy allows them to hold additional energy, making them desirable for operations that need both high power and energy, such as electric cars and renewable energy systems. Because hybrid supercapacitors combine materials based on carbon and nickel hydroxide, they have longer cycle lives. The reversible redox processes of nickel hydroxide and the stable charge storage system of lithium-ion batteries both prolong the device's lifespan [27]. Fast charging and discharging rates allow for rapid energy storage and release from hybrid supercapacitors based on nickel hydroxide [28]. Applications that need quick power spikes, like electric car regenerative braking, profit a lot from this feature. Nickel hydroxide-based hybrid supercapacitors are believed to be more environmentally friendly than some other energy storage technologies. Because they use aqueous electrolytes and don't contain any harmful or poisonous substances, they are a more environmentally friendly option.

## 2.4 Properties Of Nickel Hydroxide

The chemical compound known as nickel hydroxide  $\{\text{Ni}(\text{OH})_2\}$ , is made up of hydroxide ions and nickel. Through a variety of chemical reactions involving nickel salts and hydroxide ions, it is an insoluble compound that can be created. Among its many useful uses is as a precursor for the creation of batteries made from nickel, including those made of nickel-metal hydride (NiMH) and nickel-cadmium (NiCd), as well as Supercapacitors.

### 2.4.1 Structural properties of nickel hydroxide

An inorganic compound with intriguing structural properties is nickel hydroxide  $\{\text{Ni}(\text{OH})_2\}$ . To understand its behavior and applications, one must first understand its structure.  $\text{Ni}^{2+}$  and  $\text{OH}^-$  ions are what make up nickel hydroxide at the atomic level. They are arranged in a particular way. Because of its layered hexagonal crystal structure, which is made up of nickel atoms coordinated with hydroxide ions in each layer, nickel hydroxide has unique structural characteristics [29]. A three-dimensional structure is created by these layers piling on top of one another. The passage of ions and water molecules is made possible by tunnels found within the crystal structure. The behavior and uses of nickel hydroxide are significantly influenced by these structural characteristics, especially in energy storage devices like batteries and supercapacitors [30]. Nickel hydroxide has two primary polymorphs. The various crystal structures or forms that nickel hydroxide can take are known as its polymorphs. The alpha polymorph and beta polymorph of hydroxide of nickel are the two well-characterized polymorphs.

The nickel hydroxide ( $\alpha\text{-Ni}(\text{OH})_2$ ) alpha crystal structure denotes a particular configuration of atoms in the substance. The atoms of nickel (Ni) and oxygen (O) form sheets that are layered on top of one another to form this structure.

### 2.4.2 Electronic properties of nickel hydroxide

Energy storage systems such as batteries and supercapacitors can benefit from the intriguing electrical properties of nickel hydroxide, or  $\text{Ni}(\text{OH})_2$ . Below is a detailed explanation of nickel hydroxide's electrical properties. Nickel hydroxide is classified as a semiconductor due to its intermediate level of electrical conductivity between conductors and insulators [31]. The material's charge carriers (holes and electrons) can travel around due to its electronic band structure. The energy difference between the lowest state of energy in nickel hydroxide that is empty of electrons (the conduction band) and the most energy level that is populated by electrons (the valence band) is known as the band gap. Because its band gap is typically between 2-3 eV, nickel hydroxide is categorized as an indirect band gap semiconductor [32]. Nickel hydroxide can be used in processes related to charge transfer where electrons are transferred from nickel ions to hydroxide ions. The behavior of pseudocapacitance observed in nickel hydroxide-based energy storage devices is partially explained by these charge transfer events. Nickel hydroxide exhibits redox reactions, which are the reversible transition of nickel ions ( $\text{Ni}^{2+}$  and  $\text{Ni}^{3+}$ ) between their different oxidation states [33]. These redox processes enable increased energy storage in devices made from nickel hydroxide such as supercapacitors and batteries. Nickel hydroxide has a relatively low electrical conductivity when compared to metals or highly conductive materials [34]. However, the conductivity of the material can be increased by conductive additions or modifications to its composition and structure. Understanding nickel hydroxide's electrical properties is essential to maximizing its usefulness in a range of applications. By leveraging nickel hydroxide's semiconductor properties, charge transfer reactions, and redox behavior, experts can design and construct materials based on this

compound that have improved conductivity, energy storage capacity, and overall performance.

### 3. Theory/Calculation

#### 3.1 First principle calculation

The physical and electrical properties of real-world materials can be found using first-principle computation techniques. First principle computation is a method of calculation that directly estimates the physical properties of materials by utilizing fundamental physical quantities such as mass and charge, the coulomb force of an electron, etc. It is based on the concept of quantum mechanics. In other words, it avoids the requirement to incorporate adjustment factors to establish agreement between theoretical calculations and real outcomes by using the calculation's direct physical properties from the fundamental concept. Because electrons are so tiny, the principles of quantum mechanics control how they behave. Equation 4 provides a wave function that may be applied to characterize quantum particles.

$$\lambda P = h \quad (4)$$

Where  $h$  is the plank constant

##### 3.1.1 Schrödinger wave equation

To characterize the electronic structure of a system with several nuclei and electrons, the Schrödinger wave equation must be solved. The time-independent Schrödinger wave equation may be used to determine the wave function of an electron in a potential field ( $V$ ).

$$\left[ -\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \right] \Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \quad (5)$$

Equation 5 may be written as in (6)

$$H\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \quad (6)$$

Where  $h$  is the planck's constant,  $m$  is the mass of the electron,  $\nabla^2$  is the Laplacian (differential operator),  $V(\mathbf{r})$  is the potential energy, and  $E$  is the system's overall ground state energy and  $H$  is the molecular Hamiltonian.

The Hamiltonian is designed to represent a crystalline or molecular entity in a non relativistic quantum manner.

$$H = \left( -\sum_i^n \frac{\hbar^2 \nabla_i^2}{2m_e} - \sum_I^N \frac{\hbar^2 \nabla_I^2}{2M_n} - \sum_i I \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \sum_{i < j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{I < J} \frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|} \right) \quad (7)$$

$\mathbf{R}_I$  is the equilibrium position of the  $i$ -th nuclei,  $\mathbf{r}_i$  is the  $i$ -th electron position

Equation (7) can be expressed as:

$$H = T_e + T_n + V_{e-e} + V_{n-n} + V_{e-n} \quad (8)$$

Where:  $T_e = \sum_i^n \frac{\hbar^2 \nabla_i^2}{2m_e}$  is energy of  $n$  electrons of mass  $m_e$  that are in motion,

$T_n = \sum_I^N \frac{\hbar^2 \nabla_I^2}{2M_n}$  is the energy of  $N$  nuclei of mass  $M_n$  that are in motion,

$V_{e-n} = \sum_i I \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|}$  is the electron-nuclei attractive potential energy,

$V_{e-e} = \sum_{i < j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$  is the electron to electron interactive (repulsive) potential energy

$V_{n-n} = \sum_{I < J} \frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|}$  is the nucleus- nucleus repulsive potential energy.

It is extremely challenging to find an analytical answer to the Schrödinger equation for an entity containing  $N$  nuclei as well as  $n$  electrons. The equation can only be solved precisely by hydrogen atom or atoms that mimic hydrogen. In order to get the solution to the Schrodinger equation, Max Born and Robert Oppenheimer proposed a rough estimation method [35]

##### 3.1.2 Born-Oppenheimer approximation

The Born-Oppenheimer approximation methodology decouples (separates) the movement of the electrons from the motion of the nuclei by having the nuclei's velocity much slower than that of the electrons. In other words, it is assumed that the movement of the nuclei is fixed when examining the motion of the electrons in molecules. Inter nuclear distances are considered to be variables.  $T_n = 0$ ,  $V_{n-n} = \text{constant}$ , and the kinetic property of the nuclei thus becomes equal to zero. Consequently, the Hamiltonian transforms into:

$$H = T_e + V_{e-e} + V_{e-n} + V_{n-n} \quad (9)$$

$$H = H_{\text{elec}} + V_{n-n} \quad (10)$$

Where  $H_{\text{elec}}$  is the electronic Hamiltonian and is expressed as

$$H_{\text{elec}} = T_e + V_{e-e} + V_{e-n} \quad (11)$$

In light of this, the Born-Oppenheimer model provides equation (12)

$$H = T_e + V_{e-e} + V_{e-n} \quad (12)$$

In another notation, it is possible to write the Born-Oppenheimer as in equation (13)

$$H = T + V_{\text{ext}} + V_H \quad (13)$$

Where  $T = T_e$ ,  $V_{e-e} = V_H$ , and  $V_H = \text{Hamiltonian potential}$   $V_{e-n} = V_{\text{ext}}$  and is the external potential energy.

The equation (12) produced by the Born-Oppenheimer approximation maintains a fairly complicated form that includes a wave function with several electrons. The degree complexity has been considerably reduced by this approximation, but since the system's new wave function depends on  $N$ -bodies, more approximations are necessary in order to solve the Schrodinger equation.

##### 3.1.3 Approximation for Independent Electrons

Although the Hamiltonian has been effectively separated (divided) into the sum of the electronic and nuclear components, the Born-Oppenheimer approximation still has issues dealing with the effects of the system's multiple particle interactions. This flaw has made it more difficult to resolve the electronic issues. An approximation method known as the independent-electron approximation has been devised in order to get beyond the constraint of dealing with the impacts of many particles interaction in the system. It is

an approximation of the electron-electron interaction in crystal systems made up of numerous electrons and employed in complicated systems. This means that the independent-electron approximation approach uses a periodic potential  $V(r)$  to try to solve the complexed electron-electron interaction. as in equation (14)

$$[\hat{T}_{\text{elec}} + \hat{V}(r)] \Psi_k(\mathbf{r}) = E(k)\Psi_k(\mathbf{r}) \quad (14)$$

Where,  $r$  denotes the location of the electron and  $k$  the wave vector. Practically speaking, since periodicity is taken into consideration in the system, equation (14) offers an approximation route to solve many-electrons systems. The potential  $V(r)$  that explain the interactions must be understood, which made the approximation's inevitable shortcoming. This obstacle or constraint forced the development of more mathematical procedures that required the use of approximation techniques.

### 3.1.4 Method of Hartree Approximation

From the independent-electron approximation approach, the hartree approximation method offers a superior way to solve the many-electrons problem. The periodic potential  $V(r)$  is decoupled (separated) into the total of its electronic and ionic components in this approximation method. According to Hartree's assumption, each electron is aware of the other's electric field, and the other electrons are distributed uniformly as negative charges according to equation (15).

$$n(r) = -e \sum_i |\Psi_i(r)|^2 \quad (15)$$

Pauli's exclusion principle is demonstrated by the electrons in I as in equation (16). As a result, equation (17) gives a charge density description of the electron potential.

$$V_{\text{elec}} = e^2 \sum_i \int |\Psi_i(r')|^2 \frac{1}{|r-r'|} dr' \quad (16)$$

$$\text{So the potential } \hat{V}(r) = \hat{V}_{\text{ion}}(r) + \hat{V}_{\text{elec}}(r) \quad (17)$$

By inserting equation (17) into equation (14), the Hartree equation reduces to

$$[\hat{T}_{\text{elec}} + \hat{V}(r)] \Psi_i(\mathbf{r}) = [\hat{T}_{\text{elec}} + \hat{V}_{\text{ion}}(r) + \hat{V}_{\text{elec}}(r)] \Psi_i(\mathbf{r}) \quad (18)$$

Despite its usefulness, the Hartree approximation method has a number of flaws, including the influence of the antisymmetry of many electron wave equations and the correlations of many-electron interaction. To account for these shortcomings, the hartree approximation requires exact numerical approximations [36].

### 3.1.5 Approximation method using Hartree-Fock

A common approximation used to solve the many-body Hamiltonian is the Hartree-Fock approximation approach. By treating electrons as Fermions and making the wave function antisymmetric, it accounts for the Pauli exclusion principle. To make things simpler, the electrostatic interaction must also be averaged.

A Slater determinant Slater (1929) of single-electron wave functions can be used to solve the time-independent Schrödinger equation for an N-electron system in place of the wave function (r) as follows:

$$\Psi(x_1, x_2, x_3, \dots) = \frac{1}{\sqrt{N!}} \text{Det}[\Psi(x_1), \Psi(x_2), \dots, \Psi(x_N)] \quad (19)$$

In the Slater determinant, the antisymmetric requirement for electrons is satisfied. An exchange component that acts between electrons with the same spin and is provided by the following functions can be represented in a straightforward manner by doing this:

$$V_j^{\text{exc}} = -\frac{1}{2} \sum_j \int \Psi_j^x(r') \Psi_i(r') \frac{1}{|r-r'|} \Psi_j(r) d^3r' \quad (20)$$

The Hartree-Fock approximation equation is created by adding equation (20) to the Hartree approximation equation (19).

$$E_i \Psi_i(r) = [\hat{T}_{\text{elec}} + \hat{V}_{\text{ion}}(r) + \hat{V}_{\text{elec}}(r)] \Psi_i(r) + V_j^{\text{exchange}} \quad (21)$$

This Hartree-Fock approximation method has been demonstrated to be successful in resolving problems with adsorption and defects in solids due to the self-consistent approach to managing exchange terms [37, 38]. Another disadvantage of the Hartree-Fock technique is that it ignores the coulomb repulsion of the electrons, which is responsible for the electron correlation [39]. Because the electron velocity near the Fermi level has an unlimited value according to the Hartree-Fock approach, the approximation cannot be used to represent the density of state or other characteristics of a metallic substance.

### 3.2 Density Functional Theory

According to report by Prasad (2018)[40] and Martins (2017) [41] the density functional theory (DFT).is a computational approach that determines the number of electron in a molecule or an atom in order to deduce the attributes of the atom or molecule. The first density functional theory to be proposed was the Thomas-Fermi (TF) theory in 1927. The electronic density,  $n(r)$ , is the single input used exclusively in density functional theory. The electron-to-electron repulsion is characterized using conventional coulomb repulsion between electrons, and their kinetic energy was roughly equivalent to that of a uniform electron gas [42, 43, 44]. Wu *et al.* (2019)[45] and Witt *et al.* (2018)[46] claim that the density functional theory has evolved into a theoretical tool that has taken on a significant position among the methods used to describe and analyze the physical and chemical properties of complex systems, particularly for systems containing a lot of electrons..

The use of quantum mechanical simulations for the characterization of materials and their properties is now quite accurate and quick thanks to density functional theory (DFT). DFT converts the elements of the many-body system issue to the ground-state density function. When applying the many-bodied wavefunction in direct numerical solutions, the Schrödinger relation can be roughly approximated in large amounts of many-bodied material. However, this requires a lot of time and resources. The ground state density depends on position in a scalar way.

The first-principles method is founded on quantum mechanics, which describes the conduction of electrons and atomic nuclei in any atom or molecule [47].

### 3.2.1 Theorems of Hohenberg and Kohn

Twin theorems that Hohenberg and Kohn established in 1964 served as the foundation for density functional theory (DFT) [48].

Theorem 1:

According to the first theorem, there's a functional quantity  $F[n]$  that incorporates the kinetic energy and interaction energy for every system of  $N$  particles and every possible external potential  $V_{\text{ext}}(\mathbf{r})$ . In other words, the ground state density, among all possible electron densities, is where the total energy  $E(n)$  is lowest

$$E_0[n(\mathbf{r})] = F[n(\mathbf{r})] + \int d^3\mathbf{r} V_{\text{ext}}(\mathbf{r})n(\mathbf{r}) \quad (22)$$

$E_0[n(\mathbf{r})]$  is the ground state energy, when  $n(\mathbf{r})$  is exactly equal to the ground state electron density  $[n_0(\mathbf{r})]$ .

According to this theory, knowing  $F[n]$  and the external potential is sufficient to ascertain the ground state energy and ground state density

$$F[n(\mathbf{r})] = T[n(\mathbf{r})] + V_{\text{int}}[n(\mathbf{r})] \quad (23)$$

According to this theorem, the Hohenberg–Kohn equation can be expressed as

$$E_{\text{HK}} = T[n(\mathbf{r})] + V_{\text{int}}[n(\mathbf{r})] + \int n(\mathbf{r}) v_{\text{ext}}(\mathbf{r}) d^3\mathbf{r} \\ E_{\text{HK}} = F_{\text{HK}}[n] + \int V_{\text{ext}}(\mathbf{r})n(\mathbf{r})d^3\mathbf{r} \quad (24)$$

$E = E_{\text{HK}}$ , the exact energy of the system and  $F_{\text{HK}}$  is the universal function.

$$F_{\text{HK}} = T[n] + E_{\text{int}}[n] \quad (35)$$

where  $V_{\text{int}}$  is the internal potential for electron–electron interaction,  $T(n)$  is the energy of electron that are in motion, and  $v_{\text{ext}}(\mathbf{r})$  is the outside potential at position  $\mathbf{r}$  for the function for nuclear–electron iteration

### Theorem 2:

The second theorem defined a minimal principle for the density and said that the ground state energy of any trial electron density could never be lower than the real ground system [49]. It asserts that every system of interacting particles in an external potential  $V_{\text{ext}}(\mathbf{r})$  has a potential  $V_{\text{ext}}(\mathbf{r})$  that is solely determined by the electron density  $n(\mathbf{r})$  in the ground state, with the exception of an additive constant. One can calculate the ground-state energy by lowering the energy in relation to the electron density [41]. Two exterior potentials  $V_{\text{ext}}(\mathbf{r})$  and  $V'_{\text{ext}}(\mathbf{r})$ , if  $V'_{\text{ext}}(\mathbf{r}) - V_{\text{ext}}(\mathbf{r}) = \text{constant}$ , may coexist with the same

$$E = \langle \Psi | H | \Psi \rangle < \langle \Psi' | H | \Psi' \rangle \quad (26)$$

In the absence of degeneration, the ground state, which is presumed in the case of the Hohenberg–Kohn technique, the stringent inequality in equation (26) is valid. The final term of the equation (26) can be defined as: "ground state of  $H$ ,"

$$\langle \Psi' | H | \Psi' \rangle = \langle \Psi' | H' | \Psi' \rangle + \langle \Psi' | H - H' | \Psi' \rangle \quad (27)$$

$$\langle \Psi' | H | \Psi' \rangle = E' + \int [V_{\text{ext}}(\mathbf{r}) - V'_{\text{ext}}(\mathbf{r})]n_0(\mathbf{r}) d^3\mathbf{r} \quad (28)$$

$$E < E' + \int [V_{\text{ext}}(\mathbf{r}) - V'_{\text{ext}}(\mathbf{r})]n_0(\mathbf{r}) d^3\mathbf{r} \quad (29)$$

By considering  $E'$

$$E' = \langle \Psi' | H' | \Psi' \rangle < \langle \Psi | H | \Psi \rangle \quad (30)$$

$$\langle \Psi | H' | \Psi \rangle = \langle \Psi | H | \Psi \rangle + \langle \Psi | H' - H | \Psi \rangle \quad (31)$$

$$\langle \Psi | H' | \Psi \rangle = E + \int [V'_{\text{ext}}(\mathbf{r}) - V_{\text{ext}}(\mathbf{r})]n_0(\mathbf{r})d^3\mathbf{r} \quad (32)$$

$$E' < E + \int [V'_{\text{ext}}(\mathbf{r}) - V_{\text{ext}}(\mathbf{r})]n_0(\mathbf{r})d^3\mathbf{r} \quad (33)$$

We obtain the following contradictory equality

$$E + E' < E + E \quad (34)$$

This hypothesis has led to the inconsistency that  $E_0 + E'_0 < E_0 + E'_0$ . It implies that the external potential must be precisely defined by the ground state density (within a constant), hence dictating all system attributes

### 3.2.2 Kohn–Sham energy equation

The First Hohenberg and Kohn Statement is an existing statement that demonstrates that, in principle, the ground-state number of electron may be used to determine the electronic Hamiltonian, ground-state wavefunction, and other properties of the system, such as the ground-state energy. According to He and Sinnott (2017)[50], it doesn't specify how these traits could be acquired in any situation experienced in the real world. The ground-state energy cannot be determine, however the second Hohenberg–Kohn hypothesis suggests that the energy functional can be discovered by lowering the energy with regard to the electron density. In wave function theory, the energy is a simple function.

In 1965, Kohn and Sham provided a comprehensive and recognizable description of the many body problems, opening the way for practical DFT implementations. The Kohn–Sham (KS) equation is the Schrodinger relation for a hypothetical system of non-interacting particles that yields the same density as any real system of interacting particles. The Kohn–Sham equation is a local effective (fictitious) external potential in which the non-interacting particles travel [51].

$$\tilde{H}_{\text{aux}}^{\sigma} = -\frac{1}{2} \nabla^2 + V_{\text{eff}}^{\sigma}(\mathbf{r}) \quad (35)$$

In wave function concept, the energy is a simple function of the wave function, but in density functional theory, the precise energy functional,  $E_V(n)$ , is not known in any explicit and concrete form. DFT trades a difficult market The energy functional of the Kohn–Sham theory is written as follows:

The Hamiltonian equation is divided into sums of functions that depend on the electron charge density and are expressed as

$$E_0[n(\mathbf{r})] = T_0[n(\mathbf{r})] + V_{\text{ext}}[n(\mathbf{r})] + V_{\text{elec-elec}}[n(\mathbf{r})] \\ + E_{\text{xc}}[n(\mathbf{r})] \quad (36)$$

where  $T_0$  depict the energy possessed by the system as a result of its motion, the external potential  $V_{\text{ext}}[n(\mathbf{r})]$  explain in the equation (34) is as a result of its electrostatic interactions.  $V_{\text{elec-elec}}[n(\mathbf{r})]$  is the electron to electron repulsive potential and  $E_{\text{xc}}[n(\mathbf{r})]$  exchange and correlation energy. For a single particle, the number of electron can be expressed in accordance with wave function.

$$n(\mathbf{r}) = \sum_{i=1}^N |\psi_i|^2 \quad (37)$$

the resulting motion energy can be expressed as:

$$T_0[n(\mathbf{r})] = -\frac{\hbar^2}{2m} \sum_i \langle \psi_i(\mathbf{r}) | \nabla^2 | \psi_i(\mathbf{r}) \rangle \quad (38)$$

Where  $\mathbf{r}$  is any point in a true space,  $i$  stand for the Eigen state, and  $\psi_i$  is restricted to be perpendicular. i.e

$$\int \psi_i^*(\mathbf{r})\psi_j(\mathbf{r})d\mathbf{r} = \delta_{i,j} \quad (39)$$

The energy component of the equation (37) can be written as

$$E_0[n(\mathbf{r})] = \frac{\hbar^2}{2m} \sum_i^N \langle \psi_i(\mathbf{r}) | \nabla^2 | \psi_i(\mathbf{r}) \rangle + \int V_{\text{ext}}(\mathbf{r}) n(\mathbf{r}) d^3r + e^2 \iint \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3r d^3r' + E_{\text{XC}}[n(\mathbf{r})] \quad (40)$$

Utilizing the Lagrange multiplier  $\varepsilon_{ij}$  to the perpendicular constant in equation (39) and utilizing the variational concept, equation (38) becomes:

$$\sum_{i=1}^N \int \delta \psi_i^*(\mathbf{r}) [(-\frac{1}{2} \nabla^2 + V_{\text{eff}}(r))] \psi_i - \sum_j \varepsilon_{ij} \psi_j d\tau = 0 \quad (41)$$

Since  $\psi_i$  can be handled independently, the variables in the brackets are set to zero. Consequently, the Kohn-Sham equation is now written as

$$(-\frac{1}{2} \nabla^2 + V_{\text{eff}}(r)) \psi_i = \varepsilon_i \psi_i(\mathbf{r}) \quad (42)$$

Where the effective potential  $V_{\text{eff}}[n(\mathbf{r})]$  is given by

$$V_{\text{eff}}[n(\mathbf{r})] = V_{\text{ext}}(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \frac{\delta E_{\text{XC}}[n(\mathbf{r})]}{\delta n(\mathbf{r})} \quad (43)$$

$$V_{\text{eff}}[n(\mathbf{r})] = V_{\text{ext}}(\mathbf{r}) + V_{\text{Hartree}}(\mathbf{r}) + V_{\text{EXC}}(\mathbf{r}) \quad (44)$$

The energy determined by the Kohn-Sham methodology using the non interacting kinetic energy differs from the original ground state energy. The exchange-correlation energy  $E_{\text{xc}}[n]$  is responsible for this change. Solution is desired to for the expression 'E<sub>xc</sub>[n]' which also incorporates inputs from the kinetic energy [52, 53].

### 3.2.3 Approximation techniques for Density Functional Theory (DFT)

The kinetic energy produced from non interacting motion and the ground state energy differs according to Kohn-Sham hypothesis. The energy (EXC[n]) of exchange and correlation interaction denotes this change. The exchange correlation energy can only be determined with approximations. The majority of computations are centered on a small number of the majority that is widely used approximation approaches, despite the fact that the ordinary DFT code has access to an enormous number of them. The Local density approximation, generalized gradient approximation, and the hybrid approach are in the order of approximations.

#### 3.2.3.1 Local density approximation (LDA) approach

The LDA, which was created by Kohn and Sham in 1965, was the third significant step in the development of DFT. For a generation, it served as the foundation for solid-state computations, and it is still used in some niche applications today. The LDA approach makes the assumption that the molecule's density is constant throughout and that the exchange and correlation energy (EXC) is in accordance with density at each place. According to Aurora et al. (2014)[51], the dependency is identical to that of a homogeneous electron stream and can be presented as follows.

$$E_{\text{XC}}^{\text{LDA}}[\rho(\mathbf{r})] = \int n(\mathbf{r}) \varepsilon_{\text{xc}}^{\text{hom}}[n(\mathbf{r})] d\mathbf{r} \quad (45)$$

$$\varepsilon_{\text{xc}}^{\text{hom}}[n(\mathbf{r})] = \varepsilon_{\text{x}}(n) - \varepsilon_{\text{c}}(n) \quad (46)$$

The function '  $\varepsilon_{\text{xc}}^{\text{hom}}[n(\mathbf{r})]$  ' is determine using a quantum calculation architecture at a constant electron density  $n(\mathbf{r}) = n$

Where  $\varepsilon_{\text{xc}}$  is exchange correlation electron

Although LDA computes the electronic characteristics of some systems with rather high precision, it treats the electronic structures of some materials, particularly those with

strongly correlated structures, erroneously due to their localized nature. Another approximation is required to increase LDA's accuracy [54].

#### 3.2.3.2 Generalized gradient approximation (GGA) method

The GGA technique seeks to explain the electron density's lack of homogeneity and employs information about density and its gradient at each position as stated in equation (47), in order to address the drawbacks of the LDA method.

$$E_{\text{XC}}[n(\mathbf{r})] = \int n(\mathbf{r}) \varepsilon_{\text{xc}}[n(\mathbf{r}), \nabla n(\mathbf{r})] d\mathbf{r} \quad (47)$$

Where  $\nabla \rho(\mathbf{r})$  is density gradient.

In general, the GGA outperforms the LDA in a few qualities like total energy or energy of cohesion, but it falls short in accurately describing every aspect of a semiconductor material, including its electrical characteristics.

#### 3.2.3.3 Hybrid approach

By dividing the exchange and correlation description over a close range as well as far range, the hybrid technique can handle the LDA and GGA difficulties. The equation (48) gives the hybrid technique's definition of the exchange and correlation energy

$$E_{\text{XC}}^{\text{HSE}} = \frac{1}{4} E_{\text{x}}^{\text{sr}} + \frac{3}{4} E_{\text{x}}^{\text{PBE,sr}} + E_{\text{x}}^{\text{PBE,lr}} + E_{\text{c}}^{\text{PBE}} \quad (48)$$

A hybrid is defined as the real Hartree and Fock exchange energy plus energy of exchange and correlation at density functional theory stage

### 3.3 Quantum espresso as electronic code based on density functional theory

A collection of interconnected computer software program for studies regarding electronic framework, simulation, and refinement that is named QUANTUM ESPRESSO is used to model materials and calculate electronic-structure calculations based on pseudopotentials, density-functional theory, as well as plane waves to describe electron-ion interactions

QUANTUM ESPRESSO puts in a number of techniques and algorithms designed for a scientifically achievable predicting material properties from the nanoscale, centered around the solution of the density-functional theory (DFT) problem while employing a plane waves (PWs) basis set and pseudopotentials (PPs) to represent electron-ion interactions.. The codes are built to use periodic boundary conditions allowing for effective convergence of the thermodynamic boundary for periodic yet elaborate systems like materials that are amorphous or liquids as well as the handling of infinite crystalline structures in a basic manner [55, 56].

Supercells are also utilized to treat finite systems, and the density-countercharge approach can be employed to model open-boundary circumstances if necessary [41]. Therefore, QUANTUM ESPRESSO can be applied to any supercell or crystal structure, as well as to metals and insulators. Designs for projector-augmented waves, ultrasoft pseudopotentials, and separable norm-conserving pseudopotentials can all be used to describe the atomic cores [57, 58]. In the context of



the local density approximation or generalized gradient approximation, a variety of exchange and correlation functionals are accessible. These advanced functionals, such as Hubbard U corrections, and a few meta-generalized gradient approximation and hybrid functionals are also included [59].

One of the fundamental calculations and simulations that may be done is:

- 1 The ground-state energy computation and Kohn-Sham (KS) orbitals and energies for isolated, broadened, and periodical systems
2. Comprehensive architectural improvements of the atomic positional degrees of freedom (at the microscopic level) and unit cell degrees of freedom (at the macroscopic level) [96].
3. The noncollinear magnetism and spin-orbit pairing of the magnetic or spin-polarized system's ground state [60].
4. An early stage molecular dynamics (MD), in various thermodynamical ensembles, including NPT variable-cell molecular dynamics, utilizing alternatively the Hellmann-Feynman interactions or the Car-Parrinello Lagrangian computed on the Born-Oppenheimer (BO) interface
5. The DFPT, which provides phonon dispersions and can calculate the total energy's second and third derivatives at each given wavelength, dielectric tensors, Born effective charges, infrared spectra, and Raman tensors are examples of stationary response functions, interactions between phonons-phonon and electrons-phonon
6. The positioning of saddle points as well as transition stages utilizing the nudged elastic band (NEB) technique of transition-path optimization;
- 7 Employing a scattering method, ballistic conductance within the Landauer-Büttiker concept
- 8 Creating Wannier functions that are completely confined and other correlated quantities
- 9 Computation of nuclear magnetic resonance (NMR) and electronic paramagnetic resonance (EPR) characteristics;
10. Computation of the x-ray absorption spectra at the K-edge.

The majority of the quantum espresso programs are created in fortran 77, Fortran 95. Additionally, MPI (message passing interface) libraries enable parallelization, which significantly lowers the cost of computing. For various types of calculations, there are distinct components of Quantum Espresso and these include: Plane-wave self-consistent field, car-parrinello, Phonon, Atomic, PWcond, GIPAW, XSPECTRA, Wannier90, PostProc, and PWgui are the names of these programs [61]. PWscf (plane-wave self-consistent field) will be employed for this study endeavor,

### 3.3.1 plane-wave self-consistent field (PWSCF)

Electronic-structure computations based on density-functional theory (DFT) employ the plane-wave self-consistent field (PWSCF) approach as a computational tool. It is a key part of the open-source Quantum ESPRESSO suite of tools for modeling materials and performing electronic structure computations from first principles. The electronic wave functions are expanded in terms of plane waves in the PWscf approach. When it comes to precisely representing the

electronic states in a periodic system, plane waves are a full set of basis functions. The PWSCF technique uses an iterative process to identify a self-consistent electronic ground state of the system (see Fig 1). The process requires estimating the electron density at first, which is then utilized to determine the effective potential. Next, using the updated potential, the Kohn-Sham equations are solved to get a new electron density. Until self-consistency is attained, that is, until there is no longer any discernible variation in the effective potential and electron density this procedure is repeated. The PWSCF approach utilizes pseudopotentials to describes the interaction between valence electrons and atomic cores. The calculations become less computationally expensive when core electrons are treated effectively through the use of pseudopotentials. When examining the electronic and structural properties of materials, such as solids, surfaces, and nanostructures, the PWSCF approach is frequently employed. Band structures, total energies, pressures, and other properties that are essential for comprehending and forecasting material properties can all be found out from it.

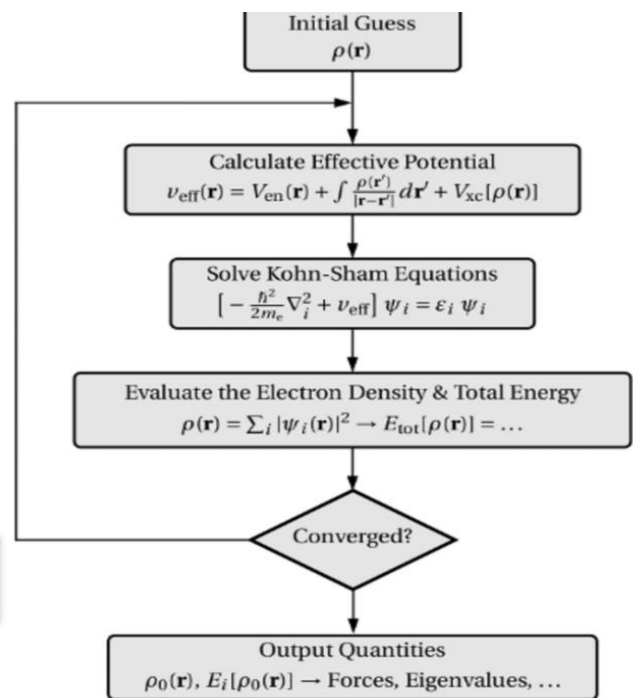


Figure 2: plane-wave self-consistent field (PWSCF) iteration scheme

## 4. Methodology

First-principle Calculation was done by utilizing density functional theory within the quantum Espresso (QE) code. According to Marx and Hutter (2017)[62], Quantum ESPRESSO is a unified software program or computer package utilized in structural characterization of materials based on density functional theory. The forces acting on the material are calculated using the Quantum Espresso software, which then makes very small adjustments to the initially estimated density in each electronic step. Plane wave basis set with kinetic cutoff of 60Ry for charge density and 480Ry for potential were used to expand the wave function along a linear combination of plane wave.

Norm conserving pseudopotential was used to replace the core electrons in order to reduce the number of wave functions. Local density approximation method within the plane wave self consistent field (PWscf) was used to describe the electrons' exchange and correlation interaction.

The nickel hydroxide structure was first examined using the XcrySDen program, which was also utilized to measure the angles and inter-atomic distances. To achieve a steady structure, structural optimization of nickel hydroxide was carried out. In this technique, the initial coordinates of the atoms were relaxed to minimize the total energy of the system. The structural optimization was performed in two ways; Relax and VC-relax (variable cell relax) optimization. The 'Relax' optimization ('relax') is used in performing geometry optimization for a given Ni (OH)<sub>2</sub> structure. The methods relax only the atomic positions while the cell parameters remain fixed. It is used to find the minimum energy and equilibrium geometry of the system. The VC-relax optimization on the other hand is used to perform the variable cell geometry optimization. In this optimization option, the atomic positions as well as the cell parameters are adjusted to minimize the total energy. Structural optimization of Ni(OH)<sub>2</sub> was performed to relax the structure in respect to the atomic position, stress and strain in order to reduce computational cost while maintaining accuracy.

After the structural optimization, a self consistent field (scf) calculation was performed using 12x12x5 k-point for the proper sampling of reciprocal space. The self consistent field calculation is to get the lowest energy wave function. The wave function provides information about the electronic structure of the material such as; positions and energies of occupied and unoccupied molecular orbital. These information can be used to calculate charge distribution, electronic transition energy, potential energy of the system. It start with initial guess for the molecular orbitals and the process is repeated until a self consistent solution is achieved (i.e until the molecular orbitals are converged and no further change are observed). The band parameters, including the bandgap, Fermi energy, etc., were then calculated using the band structure, also known as the non-self consistent field (nscf). In this calculation, the electronic density is kept fixed while calculating the band structure such as the band gap energy. The input file for the calculation of density of state (DOS) contained some parameters, including the atomic position and species in the non-self consistent field (nscf). In other words, self consistent field (scf) and non-self consistent field (nscf) needed to be conducted before density of state (DOS) could be completed.

## 5. Result and Discussion

Results of the calculation carried out on the electronic and structural properties of nickel hydroxide using density functional theory are presented and discussed in this chapter. Extracted parameters from density functional theory calculations are further analyzed to obtain parameters required to evaluate the performance of Nickel hydroxide in the application of hybrid supercapacitor.

Table 1 shows the extracted results from density functional theory calculations performed on nickel hydroxide {Ni(OH)<sub>2</sub>}. The results are extracted with respect to the application requirements in hybrid supercapacitors.

**Table 1:** Calculated results from Density Functional Theory (DFT)

Parameters	Values	Units
Lattice parameter	5.8795	Atomic unit (a.u)
Number of atom per cell	5	-
quantity of electrons	32	-
amount of Khon-Sham states	20	-
Final energy of the system	-427.7155769090	Ry
Total force on the system	0.000255	Kgm <sup>-2</sup>
Fermi energy	4.7402	Ev
Working potential	1.56	Volt(v)
Energy bandgap	3.898	eV
Valency (n)	25	-
Molecular weight	92.704	Gmol <sup>-1</sup>

It can be seen from table 1 that that lattice parameter (a) which is the atomic distance of the crystal structure of Nickel hydroxide has layer distance of 5.8795 a.u, indicating high inter-layer distance which enhances high ions diffusion rate. The final ground state energy of -427.7155769090eV shows that the crystal is stable. And the working potential of 1.56Volts is an indication of the improved specific capacitance. At absolute zero temperature, the greatest occupied energy level of electrons is known as the Fermi energy. A comparatively high density of states close to the Fermi level, shown by Fermi energy of 4.7402 eV, may improve the material's electrical conductivity. Supercapacitors benefit from this as increased conductivity makes charge transfer more effective during the quick cycles of charging and discharging. In a hybrid supercapacitor, a total force of 0.000255 Kgm<sup>-2</sup> acting on the material indicates ideal conditions for ion diffusion, structural integrity, and electrochemical performance, all of which enhance the supercapacitor's efficiency and dependability and make it a viable choice for energy storage applications.

Table 2 shows some constants applied for the parameters used to evaluate the performance of nickel hydroxide in hybrid supercapacitors.

**Table 2:** some constants employed to calculate the parameters used for Nickel hydroxide performance evaluation

Constants	Symbols	Value	Units
Relaxation time	$\tau$	$10^{-14}$	Second (s)
Electronic charge	E	1	Ev
Mass of electron	$M_e$	$5.489 \times 10^{-4}$	Atomic mass unit (a.m.u)
Faraday constant	F	96485.3321	C

## 5.1 Performance Evaluation Of Nickel Hydroxide As Hybrid Supercapacitor Electrode Material

The efficiency of hybrid supercapacitor is measured by the usage of specific capacitance, energy density, and power density. In this work, various quantities to assess the effectiveness of Nickel hydroxide as hybrid supercapacitors' electrode material were determined from the results obtain in density functional theory calculations shown on table 1 and some constants values shown on table 2.

### 5.1.1 Specific capacitance of Nickel hydroxide

The specific capacitance is a crucial factor that is employed to calculate the electrical energy density of electrochemical energy storage devices. The specific capacitance of Nickel hydroxide is obtained from the relation shown in equation 4

$$C = \frac{nF}{MV} \quad (49)$$

Where F is Faraday constant, M is the molecular weight of Nickel hydroxide, n represents the quantity of charge transfer during redox reaction, V is the operational voltage, In nickel hydroxide, a total of 2 charge are transfer, n = 2

### 5.1.2 Energy density of Nickel hydroxide electrode material

One of the parameters that determine the efficiency of electrical energy storage device is the amount of energy content . The electric energy density of nickel hydroxide is obtained using equation 50

$$E_{\text{density}} = \frac{0.5 \times C \times V^2}{3.6} \quad (50)$$

V stands for operating voltage and the specific capacitance is represented by C,

### 5.1.3 Power density of Nickel hydroxide

The power density is another parameter that is deployed to assess the effectiveness of hybrid supercapacitor. In this work, power content is obtained using equation 51

$$P_{\text{density}} = \frac{ne \times a^2}{3.6} \quad (51)$$

Where, n represents the number of valency electrons are produced by DFT calculation, 'a' represents the lattice parameter, e is the electronic charge in electron volt (eV) i.e e = 1ev

The results of the various calculations for the performance evaluation of nickel hydroxide is shown on table 3

**Table 3:** Results of the performance Evaluation Of Nickel Hydroxide

Evaluation parameters	Value	Units
Capacitance	1334.35	Fg <sup>-1</sup>
Energy Density	450.89	Whkg <sup>-1</sup>
Power Density	240.06	Wkg <sup>-1</sup>

From the Table 3, it can be ascertained that Nickel hydroxide is a viable material for hybrid supercapacitors application due to a high specific capacitance of 1334.35Fg<sup>-1</sup>, extremely high energy density of 450.89 Whkg<sup>-1</sup> and power density of 240.06Wkg<sup>-1</sup>. These results are well compare with results from other redox couple use to improve hybrid

supercapacitors. Tuyen *et al*(2017)[63] reported that structured layered of Nickel hydroxide in cobalt hydroxide{Ni(OH)<sub>2</sub> in Co(OH)<sub>2</sub>} film fashioned by utilizing electrical deposition as charge storage electrode for hybrid supercapacitor exhibited a specific capacity of 762Cg<sup>-1</sup> accompanied by an energy density of 101.3Whkg<sup>-1</sup> and specific power of 0.2Wg<sup>-1</sup>. Prakas *et al* (2021)[64] published a large specific capacitance of 1656.6Fg<sup>-1</sup> and at the same time energy density of 82.83Whkg<sup>-1</sup> and power density of 300Wkg<sup>-1</sup> with the usage of MnCo<sub>2</sub>O<sub>4</sub>@Ni(OH)<sub>2</sub> as battery electrode placed inside electrolyte of KOH/K<sub>3</sub>[Fe(CN)<sub>6</sub>]. In a similar way, Huang *et al* (2018)[65] reported on the use of redox active electrolyte of quinones and hydroquinones in a hybrid supercapacitor to reduce the diffusion kinetic and capacity imbalance issues. The redox active electrolyte provides a reversible faradic reaction to store energy and maintain charge balance between the positive and negative electrodes. They reported energy density of 26.3Whkg<sup>-1</sup> and power density of 1145Wkg<sup>-1</sup>. These results show that Nickel hydroxide is an outstanding candidate for hybrid supercapacitors.

## 6. Conclusion and feature scope

The study concludes that nickel hydroxide has a great deal of promise for hybrid supercapacitor use based on the theoretical evaluation of its energy and power density. Nickel hydroxide has good electrochemical properties, such as high specific capacitance (up to 1334.35Fg<sup>-1</sup>) and excellent cycling stability, which are essential for improving the performance of energy storage devices. Furthermore, nickel hydroxide is positioned as a promising contender for a variety of applications, including electric cars and renewable energy systems, due to its capacity to attain an appropriate balance across energy density (450.89Whkg) and power density (240.06Wkg<sup>-1</sup>). The results highlight the need for more study in this field in order to fully use nickel hydroxide's potential in supercapacitor innovation.

Looking ahead, nickel hydroxide in hybrid supercapacitor applications presents a number of intriguing study and development opportunities: Examining the implications of doping or creating composites with other materials (such carbon-based materials) in order to improve conductivity and performance, investigating cutting-edge electrode topologies to increase surface area and enhance ion transport, such as nanotechnology or three-dimensional topologies, Building and assessing novel electrolyte compositions that may improve nickel hydroxide supercapacitors' ionic conductivity and stability.

### Data Availability

The data supporting the study's findings on the energy and power density of nickel hydroxide for hybrid supercapacitor applications may be accessed by readers through Study articles, Though it offers insightful information, the theoretical evaluation of nickel hydroxide's energy and power density for hybrid supercapacitor applications has a number of limitations that should be noted: (1) The study uses computational models and simulations, which does not

adequately represent the complex nature of electrochemical activity in the actual world. Confirming that the theoretical predictions requires experimental validation. (2) Not all pertinent factors influencing energy and power density, such as temperature variations, humidity, and long-term cycle stability, studied included in the evaluation. These factors have a big impact on how well supercapacitors work in real-world applications.

### Conflict of Interest

The author declare that there is no conflict of interest

### Funding Source

None

### Author's Contribution

The author contributed 100 percent from conception stage to conclusion of the study

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**AUTHORS PROFILE**

**Umoru Efemena Sunday** earned his B.Sc in physics from University of Benin, Benin City in 2011, M. Sc in theoretical condensed matter physics from Federal University of Petroleum Resource, Effurun in 2023., and PhD in theoretical condensed matter physics from Federal University of Petroleum Resources, Effurun in View. He is currently working as Assistant Lecturer in Department of Natural Science from NINLAN, Aba since 2020.. He has published several research papers in reputed international journals. His main research work focuses on energy storage, energy conversion, computational physics, material properties. He has 15 years of teaching experience and 4 years of research experience.

