

DISCOVERING THE POTENTIAL OF NiO: A FIRST-PRINCIPLES DFT STUDY ON ANODE PROPERTIES FOR LITHIUM-ION BATTERIES

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Abstract

Transition metal oxides such as nickel oxide (NiO) are receiving significant research attention as potential anode materials for lithium-ion batteries (LIBs). The structural and electronic properties of NiO are calculated using density functional theory (DFT) method. The computed lattice parameters are in close agreement with experimental values, showing the precision of the GGA-PBESol functional compared to LDA and GGA-PBE functionals. The indirect band gap of NiO calculated using GGA-PBESol+U with $U = 8$ eV is approximately 3.84 eV, matching well with experimental values ranging from 3.60 to 4.47 eV. The density of states (DOS) analysis reveals hybridization between O 2p and Ni 3d orbitals, suggesting improved lithium-ion diffusion pathways. The bond population analysis indicates weak ionic bonding with a value of 0.32 to 0.50, leading to mechanical stability during lithium intercalation. These findings show the usefulness of NiO as an anode material in LIBs. However, the poor electronic conductivity of NiO remains a limitation, which could be solved through strategies such as compositing with conductive materials or doping. Future research should focus on optimizing these strategies to further enhance the electrochemical performance of NiO-based anodes.

Keywords: Anode materials; DFT calculations; Electronic properties; Lithium-ion batteries; NiO

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Introduction

In recent years, the development of renewable and efficient energy resources has been one of the largest global challenges for portable electronic devices and electric vehicles. New energy has received more and more attention with the increase of global pollution caused by fossil fuels. Lithium-ion batteries (LIBs) are widely used due to their stability, long cycle life and low cost. However, the capacity of traditional graphite anode materials (372 mAh/g) cannot meet the requirements of LIBs for higher energy density (Kato *et al.*, 1993). Therefore, it is necessary to find alternative anode materials with higher capacity and longer cycle performance.

In the past decades, many two-dimensional (2D) materials such as graphene and graphene-based materials, silicene, germanene, blue/black phosphorene, transition-metal carbides and carbonitrides (MXenes), transition-metal dichalcogenides (TMDCs) and h-BN have been widely investigated as the anode materials of LIBs by both theoretical and experimental studies, which provided many significant hints to optimize the electrochemical performance of electrode materials further (Ye *et al.*, 2021). The 2D materials are promising due to their large surface area and unique structure, which facilitate lithium insertion and mitigate volume changes during charging and discharging. Other materials such as borophene, phosphorene and carbon nanoparticles with high specific capacities and fast rate capability have also been widely investigated. However, their poor structural and interfacial stability will cause a severe volume change and internal deformation of electrode material, which is unsafe for battery life.

In recent years, transition metal oxides (TMOs) have been considered one of the most promising candidates for anode materials (Azad *et al.*, 2024). TMOs have high theoretical specific capacity and excellent safety performance and have been widely used in LIBs. Among all, nickel oxide (NiO) is a promising LIB anode material due to its high capacity (718 mAh g⁻¹), cost-effectiveness and environmental benefits. The density of NiO is 6.81 g/cm³, which is three times higher as compared with graphite at 2.26 g/cm³ (Li *et al.*, 2011). The theoretical energy density of NiO is about 5.8 times higher than graphite anode (Varghese *et al.*, 2008). Moreover, NiO offers unique electrical, magnetic and optical properties.

In the past two decades, computational methods have advanced significantly. The first-principles density functional theory (DFT) approach has become a powerful tool for atomistic simulations of material properties (Xiang *et al.*, 2018; Zhang *et al.*,

2019; Gao *et al.*, 2021; Zeng *et al.*, 2021; Feng *et al.*, 2022; Park and Fatima, 2023; Wang *et al.*, 2024). These are essential for understanding battery processes via the lithium-ion battery (LIB) properties predictions (Urban *et al.*, 2016; Sazman *et al.*, 2023). In this work, DFT-based computational studies are employed to investigate the structural and electronic properties of bulk NiO, aiming to evaluate its potential as an anode material for LIBs.

Computational Method

The method in this work is based on the first-principles study within density functional theory (DFT). The first-principles calculations in this work were performed using the Cambridge Serial Total Energy Package (CASTEP) (Clark *et al.*, 2005) module in Materials Studio (MS) software, which is developed and distributed by BIOVIA (formerly Accelrys). The exchange-correlation functional from local density approximation by Ceperley and Alder (Ceperley and Alder, 1980) as parametrized by Perdew and Zunger (Perdew and Zunger, 1981) (LDA-CAPZ) and generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE) (Perdew *et al.*, 1996) and Perdew-Burke-Ernzerhof for solids (GGA-PBEsol) (Perdew *et al.*, 2008) were adopted. The pseudopotentials and plane-wave basis set were employed to calculate the structural and electronic properties of NiO. The Ni 3d⁸ 4s² and O 2s² 2p⁴ of NiO were treated as valence states. The wave function for valence electrons was expanded using a plane-wave basis set within a specified cut-off energy of 380 eV. The Monkhorst-Pack scheme k-points were set as 4×4×4. The steps for the computational method start with building the crystal structure of NiO. After that, the structure was undergo geometrical optimization to find the most stable atomic arrangement by minimizing the total energy of the system. From this geometrical optimization, the data for structural properties can be obtained. For geometrical optimization, the energy change, maximum force, maximum stress and maximum displacement were set for 5×10⁻⁶ eV/atom, 0.01 eV/Å, 0.02 GPa and 5×10⁻⁴ Å, respectively. Then, calculations such as band structures, density of states and electron density were performed. The DFT+U correction was performed on both O 2p and Ni 3d orbitals to correctly produce the band gap that is in fair agreement with the experimental band gap. Lastly, the data from the calculations were analyzed using CASTEP analysis when the calculations have been completely successful.

Results and Discussion

3.1. Structural Properties

Figure 1 illustrates the crystal structure of cubic NiO (Fm-3m space group, no. 225). All calculations are performed for the antiferromagnetic (AFM) phase. The AFM phase is found to be the most stable state when compared to ferromagnetic (FM) and non-magnetic (NM) phases (Cinthia *et al.*, 2015). The lattice parameters ($a = b = c$) of NiO are around 4.10 Å for all methods from LDA-CAPZ, GGA-PBE and GGA-PBEsol as listed in Table 1. The LDA parameters underestimate about 1.70% compared to experimental data (4.17 Å), while GGA-PBE overestimates about 1.58%. Among exchange-correlation functionals, lattice parameters from GGA-PBEsol are in good agreement with the calculation result from experimental work. In comparison, lattice parameters from other theoretical work using different software are also listed, which are consistent with data in this work. The cubic structure and electronic properties of NiO can influence how Li ions interact with and diffuse through the material. A stable cubic structure can provide consistent interstitial sites for lithium-ion insertion and removal, enhancing the reversibility of anode and cycle life (Singh *et al.*, 2021).

3.2. Electronic Properties

3.2.1 Band Structures

At room temperature, NiO is a typical AFM insulator, however, the DFT method incorrectly predicts it to be a metal with remarkable electronic states across the Fermi level. A suitable Hubbard U for Ni 3d orbital was chosen from the plot of the energy gap with Hubbard U for $U = 1.0$ to 10.0 eV (Figure 2). The Hubbard U is needed because of the self-interaction error that makes electrons over-dispersed and band gaps are expected to be much lower than their real values (Samat *et al.*, 2019; DelloStritto *et al.*, 2023). The self-interaction error is likely the most significant problem of the LDA and GGA approaches to the exchange-correlation energy. This self-interaction can be explained as the false interaction of an electron with itself.

As an initial test, a calculation with $U = 0$ for O 2p and $U = 8$ eV for Ni 3d yielded a band gap of 1.975 eV. This result still underestimates the experimental band gap. However, the band gap increased as the U_{dNi} and U_{pO} increased. At $U = 8$ eV for both U_{dNi} and U_{pO} , the band gap falls within the range of the experimental band gap of 3.60 eV to 4.00 eV. The Hubbard $U = 8$ eV gives the correct description for the band gap of NiO, which is close to the experimental band gap (Kitchamsetti *et al.*, 2021). The indirect band gap E_g values of NiO are listed in Table 2, along with experimental and theoretical values.

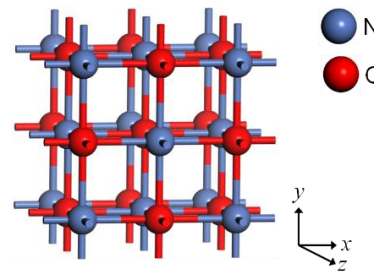


Figure 1. Crystal structure of NiO (Cubic, Fm-3m, 225)

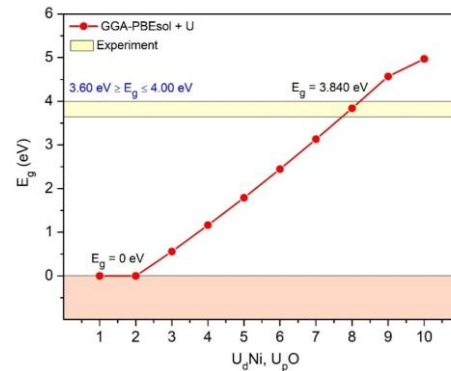


Figure 2. Variation of band gap as a function of Coulomb repulsion U_{dNi} and U_{pO} from 1 to 10 eV for NiO. This plot highlights the adjustment of the band gap values to align with experimental observation

Table 1. Lattice parameter ($a = b = c$) and volume (V) of NiO (Cubic, Fm-3m, 225) from theoretical and experiment data

Method	a (Å)	V (Å ³)	Software
LDA-CAPZ	4.099 (−1.70%)	68.87 (−5.30%)	CASTEP
GGA-PBE	4.236 (+1.58%)	76.01 (+4.83%)	CASTEP
GGA-PBEsol	4.164 (−0.14%)	72.20 (−0.43%)	CASTEP
LSDA (other work) (Ru-song <i>et al.</i> , 2018)	4.140	70.96	WIEN2K
GGA-PBE (other work) (Cinthia <i>et al.</i> , 2015)	4.213	74.78	VASP
Experiment (Benzerouk <i>et al.</i> , 2024)	4.170	72.51	-
Experiment (Siddique <i>et al.</i> , 2018)	4.171	72.56	-

The band structure calculations are reported to get information about the electronic properties of NiO. The band structures of NiO with and without Hubbard U are shown in Figure 3. The Fermi levels are indicated by dotted horizontal lines. It is found that the nature of the band gap is indirect. The indirect band gap of ~ 3.80 eV suggests that pure NiO has limited electronic conductivity. However, in an anode material, poor conductivity is generally a drawback, as it can lead to higher internal resistance. Strategies like compositing NiO with conductive materials (e.g. carbon) or doping could mitigate this by enhancing conductivity and overall battery efficiency (Le *et al.*, 2024; Mishra *et al.*, 2024).

3.2.2 Density of States

Figure 4 and Figure 5 present the total and partial density of states for NiO, calculated using GGA-PBEsol and GGA-PBEsol+U, respectively. As we can see, the O 2p states hybridize with Ni 3d states and the DOS of Ni 3d states mainly results from $d_{-t_{2g}}$ orbitals, lying below d_{-e_g} orbitals, occupying the valence band below Fermi level (Rusong *et al.*, 2018). The total density of states for NiO is completely symmetric in majority and minority spins. This indicates that the electrons occupy the majority and minority spin states equally, resulting in zero total spin moment (Cinthia *et al.*, 2015). The PDOS from GGA-PBEsol+U shows a more pronounced separation between the valence and

Table 2. Band gap (E_g) values of NiO from GGA-PBEsol, GGA-PBEsol+U and experimental band gap

Method	E_g (eV)
GGA-PBEsol	0
GGA-PBEsol+U ($U = 8$ eV)	3.84
Experiment (Shi <i>et al.</i> , 2021)	3.65 to 3.74
Experiment (Kitchamsetti <i>et al.</i> , 2021)	4.07
Experiment (Siddique <i>et al.</i> , 2018)	4.47
Experiment (Makhado <i>et al.</i> , 2024)	3.60 - 4.00

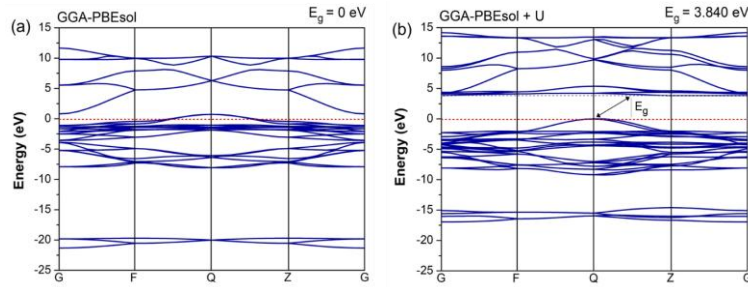


Figure 3. Band structures of NiO from (a) GGA-PBEsol and (b) GGA-PBEsol+U

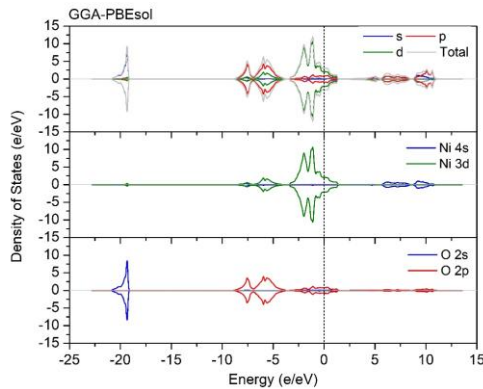


Figure 4. Total and partial density of states (DOS) for NiO, showing hybridization between Ni 3d and O 2p states from GGA-PBEsol

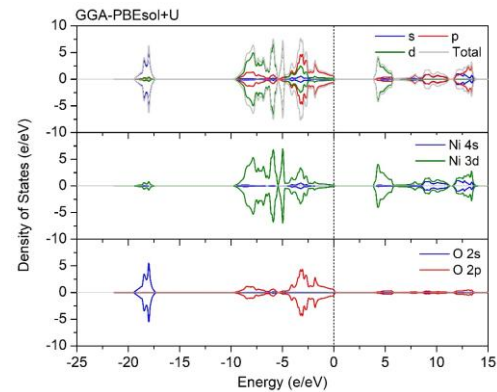


Figure 5. Total and partial density of states (DOS) for NiO, showing hybridization between Ni 3d and O 2p states from GGA-PBEsol+U

conduction bands, resulting in a band gap closer to the experimental range. The hybridization of O 2p and Ni 3d states, as seen in the density of states (DOS), suggests strong interactions between oxygen and nickel atoms. This hybridization can impact lithium diffusion pathways within the material, potentially providing multiple paths or reducing diffusion barriers, which could enhance the rate capability and charge/discharge efficiency.

3.2.3 Bonding Characteristics

The electron density maps of NiO, calculated using both GGA-PBEsol and GGA-PBEsol+U, provide valuable insights into the bonding characteristics and electronic distribution within the material. Figure 6 illustrates the electron density distribution parallel to the x and y direction. The red regions indicate high electron density and blue regions indicate low electron density. The electron density distribution around the Ni and O atoms shows a relatively uniform spread, with a weak ionic bonding character, indicated by the bond population analysis as shown in Table 3. This also reveals a degree of covalent character, as evidenced by the overlap of electron density between Ni and O atoms. When the GGA-PBEsol+U method is used, the electron density distribution changes slightly where the electron density around the Ni 3d orbitals is more localized, highlighting the ionic nature of the Ni-O bond. However, there is still some overlap of

electron density between Ni and O atoms, meaning the bond still has some covalent character. This bonding nature could impact the mechanical properties of NiO, potentially making NiO more resilient to volume expansion and contraction during lithium intercalation. This stability could lead to improved cycle life by minimizing structural degradation over time.

Conclusion

In conclusion, the fundamental properties of NiO are investigated through the first-principles calculations. The structural and electronic properties of NiO are studied using GGA-PBEsol and GGA-PBE+U methods. The calculated lattice parameters of NiO are in good agreement with the other theoretical and experimental results. The calculated structural parameter from GGA-PBEsol is in better agreement with the experimental data compared with LDA-CAPZ and GGA-PBE. The indirect band gap E_g of NiO from GGA-PBEsol calculation underestimates the band gap values. Thus, the GGA-PBEsol+U calculation is used to improve the band gap values to a greater extent. The suitable U value is selected from $U_d\text{Ni}$, $U_p\text{O} = 8$ eV. The calculated band gap of NiO using GGA-PBEsol+U has an indirect band gap of about ~ 3.80 eV. Both the valence band (VB) and conduction band (CB) contain the contributions from O 2p and Ni 3d, indicating hybridization between these states as observed from the density of states (DOS). The bond population from the electron density map shows the weak ionic characteristic. The results from the DFT calculations describe the structural and electronic properties of NiO in the cubic phase with some discussion about how these properties are useful in discovering NiO as one of the anode materials for lithium-ion batteries.

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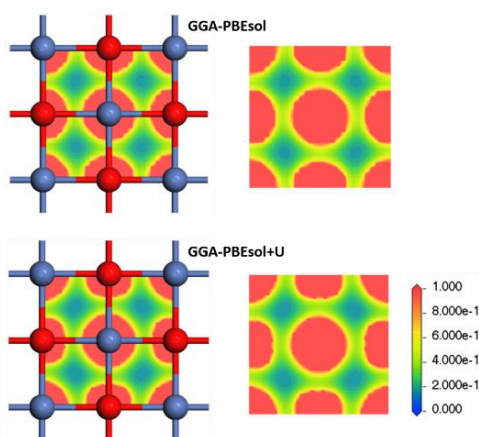


Figure 6. Electron density maps of NiO from GGA-PBEsol and GGA-PBEsol+U. The color scale represents electron density, with red indicating high density and blue indicating low density

Table 3. Indicator of population analysis for electron density

Bonding Characteristic	Ionic	Weak Ionic	Weak Covalent	Covalent
Bond Population	0 - 0.32	0.32 - 0.50	0.50 - 0.75	0.75 - 1.0

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