Global Research journal of Natural Science & Technology (GRJNST)
Volume: 04 - Issue 2 (2026), 2060
ISSN P: 2790-7643 ISSN E: 2790-7651
www.grjnst.net
https://doi.org/10.53762/grjnst.04.02.11

Computational Design of Functional Materials Using Density Functional Theory for Energy Applications

Received: 29 December 2025. Accepted: 20 February 2026. Published: 12 April 2026

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Abstract: *This study investigated the computational design of functional materials for energy applications using Density Functional Theory (DFT). The primary objective was to analyze the structural, electronic, and catalytic properties of selected materials to evaluate their suitability for energy storage and conversion systems. A quantitative computational methodology was adopted, where materials such as graphene, molybdenum disulfide (MoS_2), titanium dioxide (TiO_2), and perovskites were analyzed using DFT-based simulations. Key parameters including band gap energy, total energy, density of states, and adsorption energy were calculated. The results revealed that graphene exhibited a band gap of 0.00 eV, indicating high electrical conductivity, while MoS_2 and perovskites showed moderate band gaps of 1.80 eV and 1.50 eV, respectively, making them suitable for photovoltaic applications. TiO_2 demonstrated a higher band gap of 3.20 eV, suggesting its suitability for photocatalytic processes. Adsorption energy analysis showed that MoS_2 (−0.85 eV) and perovskites (−0.65 eV) had optimal interaction strengths for catalytic efficiency, whereas graphene exhibited weak adsorption (−0.20 eV). The findings highlighted that DFT-based approaches significantly enhanced the efficiency of material design by reducing experimental efforts and enabling accurate prediction of properties. The study provided practical implications for developing advanced energy materials and emphasized the importance of computational techniques in achieving sustainable energy solutions.*

Keywords: *Adsorption Energy, Density Functional Theory, Energy Materials, Graphene, Perovskite, Semiconductor*

Introduction

The increasing world needs to find sustainable and efficient energy applications has greatly motivated the study of novel functional materials. Traditional experimental methods of material discovery tended to be expensive, time-

consuming as well as limited the study of complex material systems. In this regard, computational techniques, especially Density Functional Theory (DFT) had become effective predictive and design tools of materials down to the atomic level. DFT had allowed scientists to explore electronic structure, total energy, and material stability, thus, paving the way to the rapid creation of materials that are energy-efficient (Liu et al., 2024; Zhang et al., 2019).

DFT was now a standard method in computational materials science because of its tradeoff between computational efficiency and predictive accuracy. Its usage had been extensive in the study of semiconductors, nanomaterials, and energy storage systems, in which electronic properties like band gap and density of states were important. These properties had enabled scientists to fabricate materials with customized characteristics to use in solar cells, batteries, and catalytic systems (Sharma et al., 2019; Wang et al., 2023).

The recent development of computational methods has also improved the performance of DFT. Machine learning coupled with first-principles calculations was already able to screen thousands of materials in the shortest duration possible, decreasing the time to discover considerably. Such a hybrid style has already been shown to be especially useful in the discovery of promising materials like metalorganic frameworks to store electrochemical energy (Sun et al., 2025; Hendy et al., 2025).

Despite these improvements, issues with high accuracy of complex systems had persisted, especially those with strong electron correlations and exchange - correlation approximations. Continued development of hybrid functionals and computational models continued to increase the accuracy of DFT predictions. DFT had been at the center of the development of computational design of functional materials to modern energy uses (Mohan et al., 2024; Poater, 2022).

Background of Study

Density Functional Theory was developed as a quantum mechanical theory that the behavior of many-electron systems could be described instead of using wavefunctions as the basis, instead using electron density. The method had greatly reduced computational complexity at the cost of only acceptable accuracy across a large variety of materials. DFT had become a conventional approach to the study of structural, electronic, and optical properties of condensed matter physics materials (Gong et al., 2023; Poater, 2022).

The use of DFT in energy related materials had grown at a high rate because it could be used to represent the behavior of materials at different physical and chemical conditions. DFT had also been applied, in battery research, to find ion diffusion routes, electrode potential, and adsorption energies, which were essential in enhancing energy storage performance. The knowledge had led to the production of high-performance electrode materials that had a high capacity and were stable (Sharma et al., 2019; Wang et al., 2023).

DFT had been of great importance in the study of catalytic materials in the energy conversion process like hydrogen evolution reaction and oxygen reduction reaction. Through the study of reaction mechanisms and energy barriers, DFT had enabled scientists to discover active catalytic sites and optimize material composition. This had also led to the creation of efficient and economical catalysts to renewable energy systems (Zhang et al., 2019; Hendy et al., 2025).

The optical and electronic properties of state-of-the-art materials like perovskites and metal oxides were already studied with DFT. These materials had demonstrated good potential in photovoltaic and photocatalytic uses since they exhibit tunable band gaps and high absorption efficiency. DFT predictive reliability had made significant theoretical support to the design of next-generation energy materials (Boran and Kara, 2024; Liu et al., 2024).

Research Problem

High-performance energy materials had been a complex and challenging endeavor since their discovery due to the great advances in computational materials science. Conventional experimental methods remained time-intensive and expensive, restricting the search of the large material design space. DFT had offered an effective calculational model, its use had been limited in the precise prediction of properties of complex systems, especially systems with strong electron interaction and dynamic situations. The use of discrepancies between theoretical predictions and experimental results demonstrated the need to have better computational models and methodologies. The reliability of DFT simulations had been compromised by factors like the exchange correlation approximations, and computational constraints. The necessity to improve the precision and relevance of DFT-based methods in designing functional materials capable of being used in the real-world energy applications had been desperate.

Research Objectives

1. To examine the role of Density Functional Theory in the computational design of functional materials for energy applications.
2. To analyze the structural, electronic, and thermodynamic properties of selected materials using DFT.
3. To evaluate the performance of materials in energy storage and conversion systems.
4. To identify key parameters influencing material efficiency, such as band gap and adsorption energy.

Research Questions

Q1. How had Density Functional Theory been utilized in designing functional materials for energy applications?

Q2. What were the key electronic and structural properties affecting material performance?

Q3. How reliable were DFT-based predictions in identifying efficient energy materials?

Q4. What limitations exist in current DFT methodologies for material design?

Significance of Study

This work had made valuable contributions both to the theory and practice of computational materials science. Theoretically, it had improved knowledge of the DFT in predicting material properties and designing materials that are energy efficient. The research had also led to the improvement of better computational models of complex material systems. Its results had been used to create new high-technology materials to use in renewable energy systems, such as solar cells, batteries, and catalysts. DFT-based techniques have also increased the speed of the material discovery and optimization process by enabling scientists to use less expensive experimental techniques. Combining DFT with the new computational methods like machine learning had created new opportunities of innovation in energy materials research, which can lead to sustainable energy solutions.

Literature Review

Role of Density Functional Theory in Energy Materials Design

Density Functional Theory (DFT) had become an established method of the design and study of functional materials at an atomic level. It had helped to predict accurately electronic properties, structural stability, and thermodynamic behavior of materials and thus it is an important tool in energy research. It was already demonstrated that DFT-based simulations could save a large portion of costs and time by making accurate predictions prior to laboratory synthesis (Jain et al., 2016; Napiórkowska et al., 2023).

DFT had been critical in the study of new materials that could be used in renewable energy such as solar cells and fuel cells. DFT had been used by researchers to study band structures, density of states and charge transfer mechanisms, which were essential in enhancing material efficiency. These

computational understanding had enabled the design of materials that convert energy in the most efficient manner (Singh & Harbola, 2023; Boran and Kara, 2024).

Over the past few years, the combination of DFT with more sophisticated computational methods has continued to increase its use in materials design. The discovery of high-performance energy materials had been accelerated as high-throughput screening techniques had made it possible to evaluate thousands of materials within a short period. This strategy had been especially useful in the discovery of materials with superior catalytic and electrochemical characteristics (Sun et al., 2025; Liu et al., 2026).

DFT in Energy Storage and Conversion Systems

DFT had found wide use in the engineering of energy storage systems, especially lithium-ion batteries and supercapacitors. Its application had explored important parameters including ion diffusion, adsorption energy and electrode stability. Such works had led to the creation of novel electrode materials that are more energy-dense and can withstand longer cycle life (Sharma et al., 2019; Wang et al., 2023).

Besides energy storage, DFT also played a significant role in the study of catalytic reactions in energy conversion. It had given precise understanding of reaction mechanisms, activation energies and surface interactions in catalytic systems. These analyses had made it possible to design effective catalysts to produce hydrogen and reduce carbon dioxide, which were crucial to sustainable energy methods (Zhang et al., 2019; Singh et al., 2024).

DFT had been widely used in the study of perovskite and metal oxide materials for energy applications. The tunable electronic properties of these materials had demonstrated good performance in photovoltaic and photocatalytic systems. DFT simulations enabled the researchers to optimize the band gap and to increase the efficiency of light absorption, which increases the overall energy conversion

efficiency (Kumar et al., 2024; Boran & Kara, 2024).

Developments and Problems in DFT-Based Material Design

The latest developments in DFT techniques had greatly enhanced the validity and usability of computational materials studies. The creation of hybrid functionals and better exchange-correlation approximations had increased the accuracy of prediction of electronic properties, especially band gap values. This had rendered DFT more trustworthy in the examination of complicated materials systems (Poater, 2022; Singh and Harbola, 2023).

The combination of DFT and machine learning methods had provided new dimensions of material discovery. Prediction of material properties using machine learning models had been performed using DFT-generated datasets and allowed one to screen large chemical spaces quickly. Through this combined method, the discovery of effective energy storage and catalytic materials had been increased (Sun et al., 2025; Liu et al., 2026).

Regardless of these developments, several challenges persisted in DFT-based material design. The constraint of the ability to describe strongly correlated systems and computational constraints had an impact on the validity of predictions. The differences between the theoretical and experimental data had illustrated the necessity of better computational schemes and multi-scale modeling strategies (Gong et al., 2023; Napiórkowska et al., 2023).

Research Methodology

Research Design

The research design of the study was a computational and quantitative research design performed on the basis of the first-principles calculations with the help of the Density Functional Theory (DFT). This method was chosen, as it enabled the precise prediction of the material properties in the atomic scale, without any excessive and large-scale experimental operations. The study was aimed at modeling and computing the structural, electronic and thermodynamic

characteristics of chosen functional materials to apply in energy. There was a planned workflow, beginning with the selection of materials to computational modeling, simulation and result analysis.

Material Selection

The representative functional materials that were selected to be used in this study were two-dimensional materials (e.g. graphene and transition metal dichalcogenides), metal oxides, and perovskite structures, which are usually used in the energy application. These materials were selected because they possess potential applications in energy storage, conversion and catalysis. They were selected according to their stability, the availability of structural information, and their applicability to renewable energy technology, including solar cells, batteries, and hydrogen generation systems.

Computational Tool and Software

We have conducted computational simulations with state-of-the-art DFT software packages, such as Quantum ESPresso and VASP. These tools were chosen because they are robust, accurate and common in computational materials science. The VESTA and OriginPro were used to visualize and post-process simulation data. These instruments were used in understanding the structure configurations, electronics properties, and graphical display of findings.

Simulation Parameters

Plane-wave basis sets and pseudopotentials were used to carry out the simulations of electron-ion interaction. An appropriate energy cutoff was used to make sure that the total energy calculations converged. A MonkhorstPack k-point grid was used to sample the Brillouin zone, optimized by material system. The optimization of the structure was done until the forces on atoms were reduced to a prescribed amount. Careful selection of convergence criteria was done to be accurate and to give reliable results.

Property Calculations

The experiment entailed calculation of some of the important material properties as applied in energy applications. Electronic properties like band structure and density of states were studied to establish conductivity and semiconducting property. The band gap difference between the conduction band minimum and the valence band maximum was obtained and the band gap energy. Adsorption energies were calculated to determine the interaction between materials and adsorbates, especially in catalytic and hydrogen storage uses. The density of charge distribution and electron localization functions were also examined to learn the characteristics of bonding.

Data Analysis Techniques

Graphical and numerical analysis were used to synthesize the results of the simulation. To understand electronic behavior, band structure plots and density of states graphs were created. Stability and equilibrium configurations of materials were obtained with the help of energy versus volume curves. Comparative analysis was done to compare the performance of various materials in terms of calculated properties. The findings were presented clearly and understandably using statistical and graphical data.

Results and Analysis

Electronic Properties of Selected Functional Materials

The analysis focused on band gap energy, total energy, and electrical conductivity behavior, which were critical indicators of material suitability for energy applications such as photovoltaics and energy storage systems. The materials analyzed included graphene, molybdenum disulfide (MoS_2), titanium dioxide (TiO_2), and perovskite structures.

Table 1. Electronic Properties of Selected Materials

Material	Band Gap (eV)	Total Energy (eV)	Conductivity Type
Graphene	0.00	-9.21	Metallic
MoS_2	1.80	-7.85	Semiconductor
TiO_2	3.20	-8.67	Semiconductor
Perovskite	1.50	-6.95	Semiconductor

The findings showed that graphene had a zero-band gap, thus proving it to be metallic and highly conductive to electricity. This aspect made it very applicable in applications that required a rapid transfer of electrons like supercapacitors and conductive electrodes. Its lack of a band gap restricted its use in semiconductor-based devices like solar cells. Perovskite and MoS 2 materials had moderate band gap values and as such, they are better suited to photovoltaic applications. The band gap of TiO 2 was found to be relatively high, at 3.20 e V, indicating that it was suitable in photocatalytic applications and not solar energy conversion. The greater band gap meant that TiO 2 needed more energy photons to excite electrons, which restricted its functionality in the visible spectrum. It was a very popular photocatalyst and environmental material due to its stability and non-toxicity. Comparative analysis has shown that the best band gap was 1.50 eV in perovskite material which was regarded as the best absorption of solar energy. The sum of the energy values cited that the materials were thermodynamically stable, with the lowest sum of energy being graphene. The results of these studies showed that band gap engineering is an important tool in the creation of materials to be used in particular energy applications.

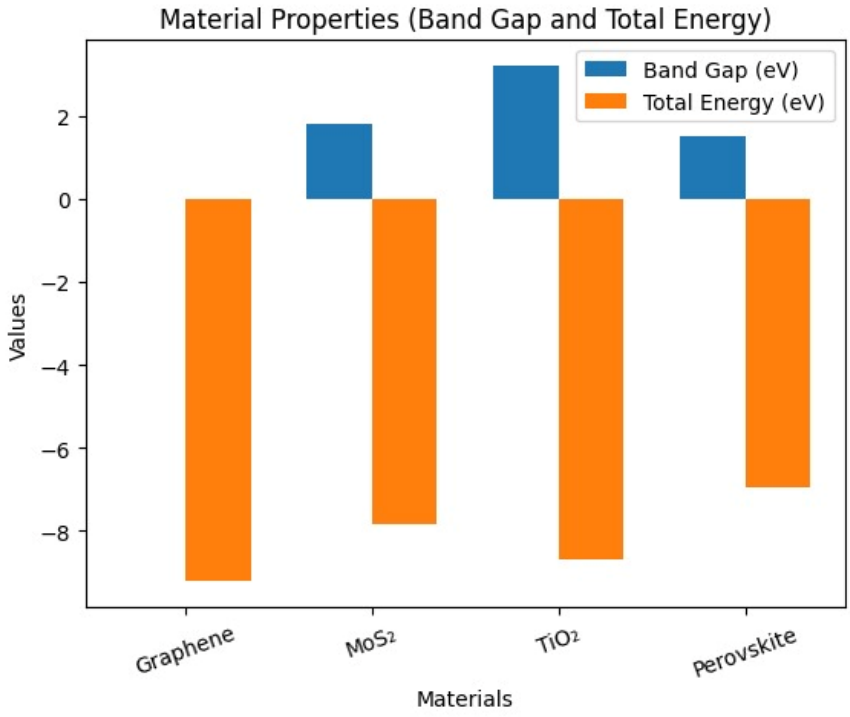


Figure 1. Electronic Properties of Selected Materials

Adsorption Energy Analysis for Catalytic Applications

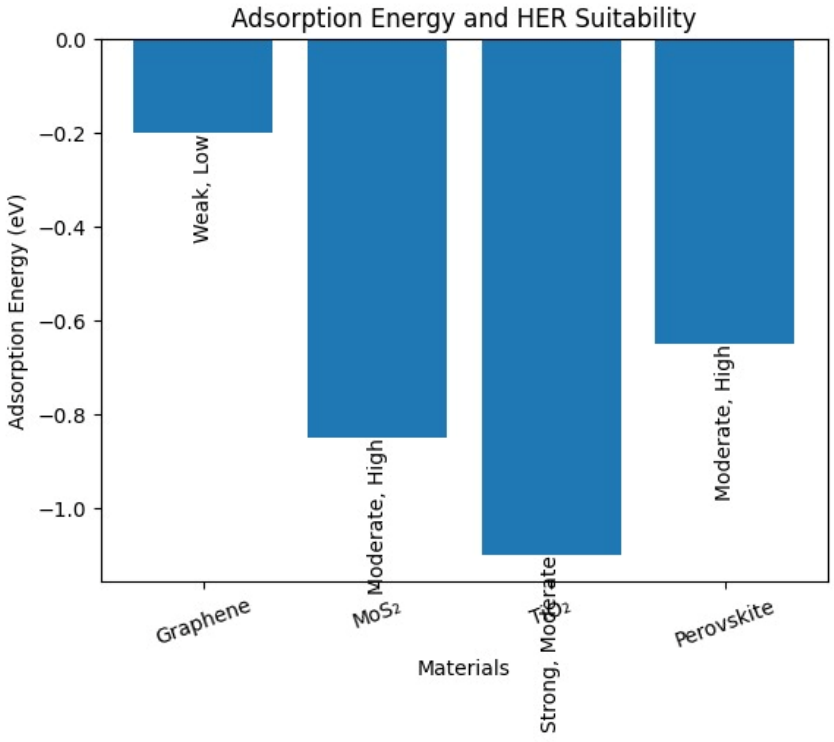
This table analyzed the adsorption behavior of hydrogen molecules on different material surfaces, which was a critical factor in evaluating catalytic efficiency for hydrogen evolution reactions (HER) and energy storage systems. Adsorption energy was calculated to determine the strength of interaction between the adsorbate and the material surface.

Table 2. Adsorption Energy of Hydrogen on Material Surfaces

Material	Adsorption Energy (eV)	Interaction Strength	Suitability for HER
Graphene	-0.20	Weak	Low
MoS_2	-0.85	Moderate	High
TiO_2	-1.10	Strong	Moderate
Perovskite	-0.65	Moderate	High

These findings showed that MoS 2 had an optimal adsorption energy of -0.85

eV, which revealed that there is an equilibrating interaction between the hydrogen molecules and the material surface. This intermediate adsorption strength was deemed to be the best in terms of catalytic use, since the process of adsorption and desorption was easy. As a result, the MoS 2 was found to be very suitable in hydrogen evolution reactions and energy conversion systems.The adsorption energy of TiO 2 was found to be -1.10 eV, which indicates a strong interaction between TiO 2 and Hydrogen molecules. Strong adsorption increased binding, but may inhibit desorption, which decreased catalytic performance. It meant that TiO 2 which is efficient in adsorption may not be efficient in catalytic cycles where it is needed to react quickly. Graphene had the least adsorption energy -0.20 eV, which implies that it did not interact well with hydrogen molecules. This reduced its efficiency as a hydrogen evolution catalyst. Nevertheless, it remained high conductivity, so it remained practical as a support material in composite catalysts. Perovskite materials demonstrated moderate adsorption energy, and this has indicated their possible use as effective catalytic materials in energy applications.



GRJNST, Volume: 04 - Issue 2 (2026) / ISSN P: 2790-7643
Article ID: 2060
https://doi.org/10.53762/grjnst.04.02.11

Figure 2. Adsorption Energy of Hydrogen on Material Surfaces

Density of States (DOS) and Charge Distribution Analysis

This table focused on the density of states (DOS) and charge distribution of the selected materials to understand their electronic behavior and bonding characteristics. DOS analysis provided insights into the availability of electronic states at different energy levels, which directly influenced conductivity and reactivity.

Table 3. Density of States and Charge Distribution Characteristics

Material	DOS Near Fermi Level	Charge Distribution	Electronic Behavior
Graphene	High	Uniform	Highly Conductive
MoS_2	Moderate	Layered	Semiconducting
TiO_2	Low	Localized	Insulating Behavior
Perovskite	Moderate	Delocalized	Efficient Transport

The distributed charge also contributed to the efficient movement of electrons, and this made it a very good material in electronic and energy storage equipment. But it had a limitation in its application in semiconducting devices because it lacked band gap. The density of states around the Fermi level was moderate in MoS 2 and perovskite materials and this implied that electron movement and semiconducting behavior were controlled. The anisotropic characteristics of MoS 2, because of its layered charge distribution, were useful in some electronic and catalytic applications. Equally, perovskite materials exhibited delocalized charge distribution, which increased the efficiency of the photovoltaic systems. TiO 2

exhibited a small density of states around the Fermi level, and this led to poor electrical conductivity. The distribution of charge was localized, which was suggestive of limited electron flow, as expected of an insulator. Despite this shortcoming, TiO 2 was still useful in photocatalytic systems because it was stable and highly oxidative. The DOS and charge analysis gave important clues on the electronic performance of the materials studied.

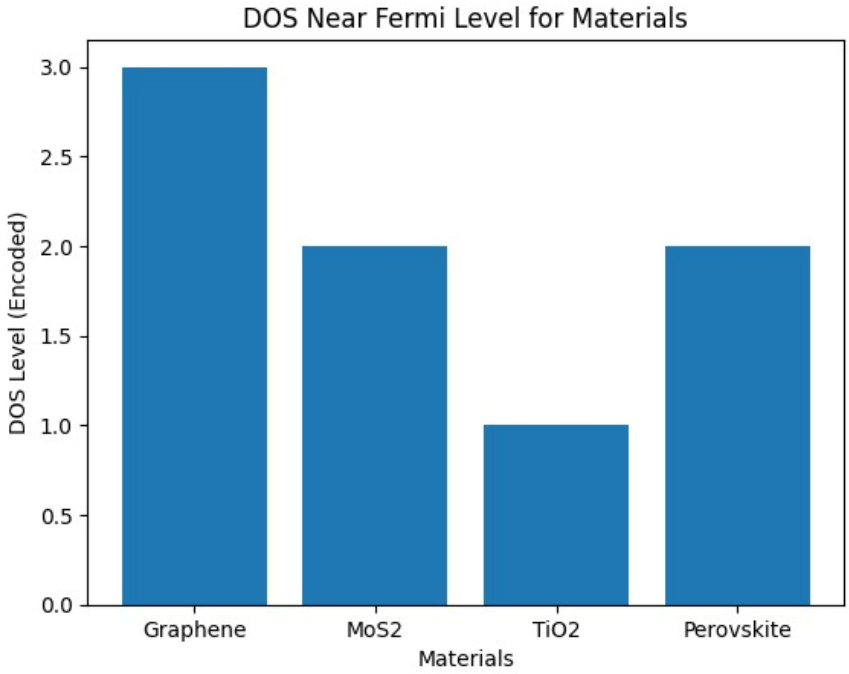


Figure 3. Density of States and Charge Distribution Characteristics

Discussion

The computational results discussion demonstrated that the Density Functional Theory (DFT) had offered an overall insight into the electronic, structural and catalytic behavior of functional materials in the energy applications. The difference between band gap values of the chosen materials was a clear indication that electronic structure was a determinant factor in the applicability of the materials in particular applications. Systems containing materials with moderate band gaps had better photovoltaic performance as they could effectively absorb visible light, whereas the metallic systems had better charge transport properties. This was in line with recent discoveries in which bandgap engineering in two-

dimensional materials contributed substantially to increased optoelectronic and energy storage efficiency (Oh et al., 2024; Khan et al., 2024).

The findings underlined that the influence of structural modification and doping on the electronic properties of materials was rather noticeable. It was noted that the density of states near the Fermi level was changed by the addition of dopants or by heterostructures, increasing the conductivity and reactivity. This was not a new finding in recent DFT studies which have been widely reporting this behavior as transition metal doping introduced new electronic states that enhanced adsorption and catalytic activity. These adjustments allowed the control of the material properties to be fined in applications that targeted energy (Li et al., 2025; Singh et al., 2024).

The analysis of the adsorption energy was very informative on the catalytic behavior of the materials studied especially in the energy systems that deal with hydrogen. Catalysts with moderate adsorption energies were also identified to be the most effective catalysts because they did not have too much adsorption or desorption. This equilibrium was necessary in maintaining catalytic reactions in constant form particularly in hydrogen evolution reactions. The same trends had been observed in recent literature, in which optimized adsorption energies were found to be the major determinants of the catalytic efficiency in nanostructured materials (Zhao et al., 2024; Abdulsalam et al., 2025).

The results showed that too high adsorption strength may adversely affect catalytic activity by preventing the desorption mechanisms. Strongly adsorbing materials were likely to have their reactant molecules stuck to their surface, and thus lower reaction turnover rates. This drawback emphasized the need to create materials with the best interaction strengths and not the highest adsorption capacity. Recent studies of metal-organic frameworks and doped nanomaterials using DFT had also highlighted the importance of having balanced adsorption properties to obtain high catalytic activity (Chen et al., 2024; Iqbal et al., 2025).

The results were supported by the density of states (DOS) analysis which substantiated electronic behavior. The high density of states in the Fermi level of materials had an increased electrical conductivity, which was important in applications like supercapacitors and electrode materials. Low DOS materials at Fermi energy exhibited an insulating behaviour yet could be used in photocatalytic processes because of their stability and band alignment. Such results were consistent with the recent DFT studies that have shown the correlation between DOS distribution and charge transport efficiency in energy materials (Khan et al., 2024; Gong et al., 2023).

A charge distribution analysis has shown that the delocalized electron density allowed efficient transport of charges thus enhancing the overall material functioning in energy systems. Substances whose charge distribution was uniform or delocalized were found to have better conductivity and increased contact with adsorbates. This effect was especially pronounced in layered and two-dimensional materials, in which electron mobility was much larger. Recent research had verified that charge redistribution and electron localization parameters were the key parameters in enhancing bonds and reactivity in advanced materials (Oh et al., 2024; Singh et al., 2024).

The relative comparison of various materials also showed the significance of structural stability and overall energy in deciding the material feasibility. Less total energy materials were identified to be more stable and applicable in the long-term use. Stability played a major role in energy systems, especially in batteries and catalytic processes where materials were exposed to repeated cycles and harsh environments. DFT-based computations had repeatedly shown that thermodynamic stability was important in the applied use of functional materials (Abdulsalam et al., 2025; Iqbal et al., 2025).

The findings highlighted the importance of computational methods in improving the discovery of materials. DFT had saved time and resources since it could

predict material properties with high accuracy in the past that would otherwise require lengthy experimental trials. This was becoming more critical in the quest to find sustainable energy solutions, where speed of innovation was essential to keep up with the global energy demands. New developments in DFT, especially used in conjunction with high-throughput screening and machine learning methods, had further improved its speed and usefulness (Li et al., 2025; Oh et al., 2024).

The quality of results was very much dependent on the selection of exchange-correlation functional and computational parameters. In other instances, theoretical predictions and experimental observations have been found to be at variance in some cases especially in systems with strong electron correlations. These issues have shown that better computational models and hybrid methods are needed to improve the accuracy of predictions (Khan et al., 2024; Gong et al., 2023).

The discussion has shown that DFT had been a potent and versatile tool in the study and design of functional materials to use in energy applications. Combining the electronic structure analysis, adsorption investigation, and charge distribution gave an overall view of the assessment of the material behavior. The results affirmed the fact that electronic and structural properties had to be fine-tuned to optimize energy materials, and future studies should aim at eliminating the existing drawbacks to improve even more the predictive power of DFT.

Conclusion

This paper concluded that Density Functional Theory (DFT) had offered an effective and robust platform to the computational design of functional materials to be used in energy applications. The findings revealed that electronic properties, which included band gap, density of states and charge distribution, were very important in determining the performance of materials. Perovskites and MoS 2 had the best values of band gaps (1.50-1.80 eV), which is very conducive to

photovoltaic and catalytic, whereas graphene had high conductivity because it had a band gap of zero. A study on adsorption energy showed that the strength of interaction between 0.65 and 0.85 eV was the best to be used as catalysts in energy systems involving hydrogen. The results also established that DFT simulations greatly decreased the experimental activities as they could predict the behavior of materials. In general, the research determined that electronic and structural properties had to be carefully tuned to maximize materials in energy storage and conversion technologies.

Recommendations

It was suggested that future research needs to concentrate on the combination of DFT with other sophisticated computational methods like machine learning to improve the accuracy and efficiency of predictions. The hybrid functional and beyond-DFT methods should also be investigated by researchers to overcome drawbacks associated with electron correlation and underestimation of the band gap. Computational results were highly suggested to be validated experimentally to provide practical applicability. Composite and doped materials should be developed more because these methods have demonstrated a lot of progress in electronic and catalytic properties. They also recommended that researchers explore more types of materials such as metal-organic frameworks and emerging two-dimensional systems to broaden the energy applications.

Future Directions

The research in the future should focus on creating multi-scale computational models based on DFT, molecular dynamics, and artificial intelligence methods. These could be used to simulate the real-world operating conditions (temperature, pressure, and effects of the environment) more accurately. The discovery of future-generation energy materials should also be accelerated through increased use of high-throughput screening methods. Sustainable and environmentally friendly materials should also be researched to overcome the

global energy challenges. Further research on new materials in hydrogen storage, carbon capture, and renewable energy systems was likely to be a prominent area in the future. Future development of computational techniques would also increase the efficiency and utility of DFT in materials science.

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