



DENSITY FUNCTIONAL THEORY STUDIES OF NANOMATERIALS WITH APPLICATIONS IN NANODEVICES: A REVIEW

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ABSTRACT

This review article studies density functional theory (DFT) properties and nanomaterials applications in the current trend. According to reviews by scientists and leading research institutions, the number of applications of density functional (DF) formalism in chemistry and materials science has increased. Through this article, our goal is to discuss in detail the properties of Density Function Theory (DFT), nanotechnology, nanomaterials, and nanodevices, how they are used, and to explain important information about Nano applications in detail. The various properties of nanomaterials (such as optical, optoelectronic, catalytic, and magnetic) show good agreement between experimental values and those predicted by DFT calculations. Scientists conducting experiments, performing DFT-based calculations alongside their experiments makes it easier to predict the properties of nanomaterials based on the physical and chemical properties obtained from the experiments. Density Functional Theory (DFT) has emerged as a powerful computational tool to model, understand, and predict different material properties at a quantum mechanical level for nanomaterials.

In this article, the author will discuss the fundamental principles of DFT and the applications of nanomaterials in nanodevices.

Keywords: DFT, nanomaterials, research, materials science, properties, tool, nanodevices etc.

INTRODUCTION

In the field of global technology, a large number of scientists and technologists from renowned companies, R&D organizations, and academic research laboratories are working diligently to develop nanotechnology by utilizing the unique properties of nanostructured materials (Nano applications and nanodevices) with high precision. Nanomaterials and nanodevices are being rapidly adopted in various fields, including medicine, industry, agriculture, and human safety devices (such as sensors and temperature devices, etc.), among others. Nano materials demonstrate the unusual physical, chemical, optical, and mechanical properties, which include, among others, larger surface areas, quantum effects, and new behaviours that emerge at the nanoscale, distinguishing them from bulk materials [1-3]. The applications of nanomaterials include the fields of information storage technology, semiconductors, microelectronics, aerospace technology, defense, biomedicine, biomedical imaging, pharmaceuticals, catalysis, petrochemicals, clean-energy sectors, new-energy resources, photonics, glass, ceramic industries, etc [4-5]. Nanomaterials are considered to be materials at nanoscale dimensions typically within the

range of 1–100 nanometers, and the criteria for classification of nanomaterials are based on dimensions, as shown in Figure 1.

Density functional theory is based on first principles and enables predictions of material properties without requiring any prior knowledge or the ability to synthesize the material. DFT Basically, the theorem proposes that a system's ground-state properties can be obtained as a functional of the electron density, and accurately predict the physical and chemical properties of systems of up to about a thousand atoms [7-8]. Density functional theories (DFTs) have played an important role in understanding these phenomena. DFT techniques also find application in many different areas of industrial research such as translation of the engineering problem, physicochemical properties and, confrontation with laboratory experiments.

Nanomaterials are categorized according to their different shapes such as nanoparticles, nanowires, nanorods, and so on depending on their type and size. Each type has its applications in different fields such as, electronics, medicine, energy, and environmental

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science etc. [9-12]. In this review article, author describe the DFT calculations for explaining and predicting the optical properties, physical, and

chemical properties of nanomaterials. The purpose of this work is to present the Density Functional Theory and its main applications in nanotechnology.

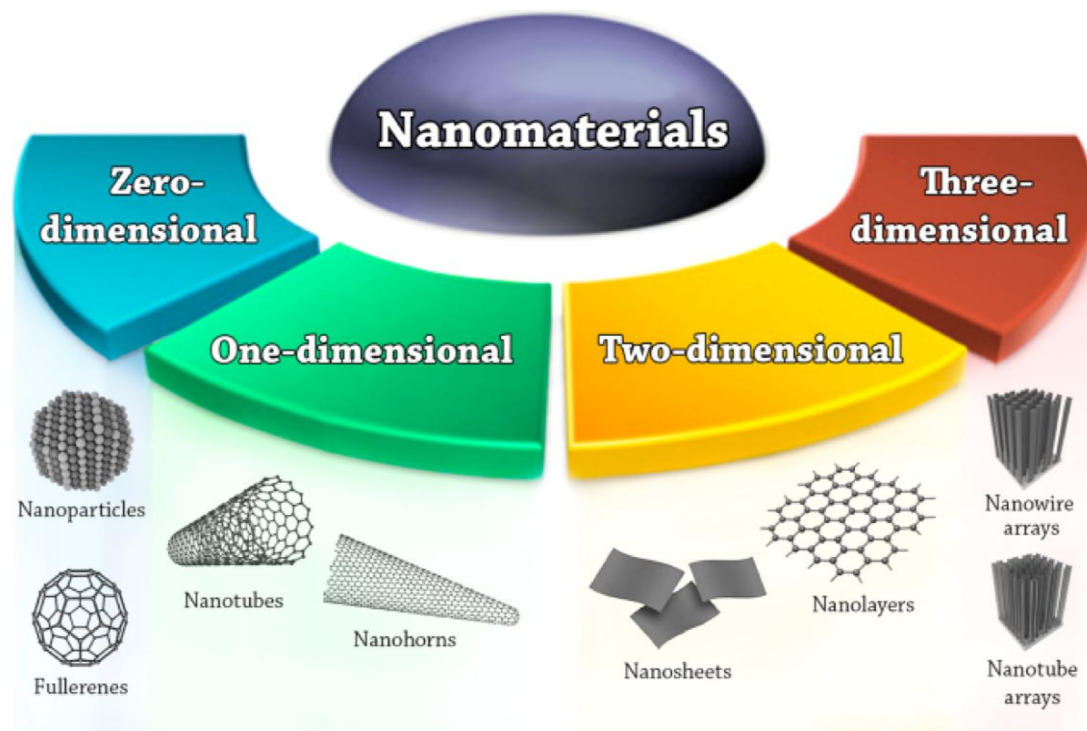


Figure 1: Nanomaterials classification based on dimensionality [6].

Theoretical background of DFT

To understand the special place of DFT in modern quantum chemical methods, it is first necessary to understand traditional wavefunction-based methods and mechanical and first-principles methods. Density functional theory (DFT) is a quantum mechanical model whose main purpose is to efficiently predict the electronic structure, stability, and properties of many body systems such as atoms, molecules, and solids by solving an approximation of the Schrödinger equation based on electron density rather than the complex wave function [13]. DFT provides a quantum mechanical modelling method that allows the investigation of the electronic structure of atoms, molecules, and solids [14]. Density functional theory approximates the total energy as a function of the electron density, making it an emerging and powerful tool for understanding and predicting various properties at the nanoscale in materials science [15]. DFT is widely used to study molecular and electronic configurations, binding energies, and material properties in physics, chemistry, and biology.

Fundamental of Density Functional Theory

Density-functional theory offers a powerful

method for calculating the ground-state total energy and electron density of a system of interacting electrons. DFT is a quantum-mechanical method for investigating the electronic structure of atoms, molecules, and solids, relying on electron density [16]. The Schrödinger equation for a many-body system may be simplified to the Kohn-Sham equation, a single-particle independent Schrödinger equation. It can be numerically solved within density functional theory [17]. The most fundamental of these approaches originates from the pioneering work of Hartree and Fock in the 1920s. The Hartree and Fock (HF) method assumes that the exact N-body wavefunction of the system can be approximated by a single Slater determinant of N spin-orbitals [18]. HF methods usually present difficulties in their application to bioinorganic and biological systems, and their cost is currently still prohibitive for molecules containing more than about 20 atoms. The concept of DFT is that, rather than depending on the wave function and needing substantial uncontrolled calculations, the characteristics of an interacting electron system will be assessed via its electron density [19].

Hybrid Fundamental of Density Function Theory

This hybrid approach significantly improves the band gap, thermochemistry, and reaction barriers, and easily corrects the self-interaction errors that occur in the approximations. Hybrid Density Functional Theory improves upon standard Kohn-Sham (KS) DFT by mixing a portion of the exact exchange energy from HF theory with the exchange-correlation energy from DFT functionals [20]. Hybrid Functionals in DFT improve accuracy by mixing standard, local Generalized Gradient Approximations (GGA) with nonlocal HF exact exchange. Developed largely by Becke (1993), this approach reduces self-interaction errors and enhances predictions of band gaps, atomization energies, and bond lengths in molecular and solid-state systems.

Fundamentals of Hybrid Functionals: Some important fundamentals of hybrid materials are given below:

- **Core Concept:** Core concept of hybrid functional are hybrid of DFT and HF.
- **The Mixing Principle:** The mixing principle in DFT refers to creating hybrid functionals by combining a portion of HF exchange energy with exchange-correlation energy from GGA.
- **Advantages:** Hybrid functionals are widely used to improve upon the limitations

of standard local density approximations (LDA) and GGA.

- **Limitations:** Hybrid functionals, which mix exact HF exchange with DFT exchange-correlation, are widely popular for improving band gaps, but they possess significant limitations.

Designing Density Function Theory Calculations for Materials Science

Designing DFT calculations for materials science involves modeling ground-state properties (bonding, structures, energies) by analyzing electron density rather than high-dimensional wave functions, significantly reducing computational costs [21]. Computational techniques of DFT design calculation of materials sciences include quantum mechanical computations, classical/molecular mechanics, mesoscale modeling, finite element analysis, and engineering design, shown in Figure 1. Material properties are calculated using corresponding physical laws, such as the Schrödinger equation in the quantum regime or Newton's laws of motion in the classical regime [23]. Functional materials are highly sensitive in one or several of their properties to changes in the environment, whereas structural materials are optimized to withstand external forces [24]. Important groups of functional materials are classified along with the challenges, as shown in Table 1.

Table 1: Classification of Selected Functional Materials with Respect to the Mechanism.

S.No.	Category	Application	Simulation Challenges
1	Electronic	Microelectronics	Doping, defects, interfaces
2	Optical	Laser diodes, light emitting diodes	Band structure, matrix elements
3	Magnetic	Storage applications, spintronics, magnetocalorics	Magnetic structure, anisotropies, disorder
4	Mechanical	Structural components, shape memory effect, piezo- and pyroelectrics	Extended defects, elastic constants, complex energy landscapes, plasticity, disorder
5	Combinations	Multiferroics	

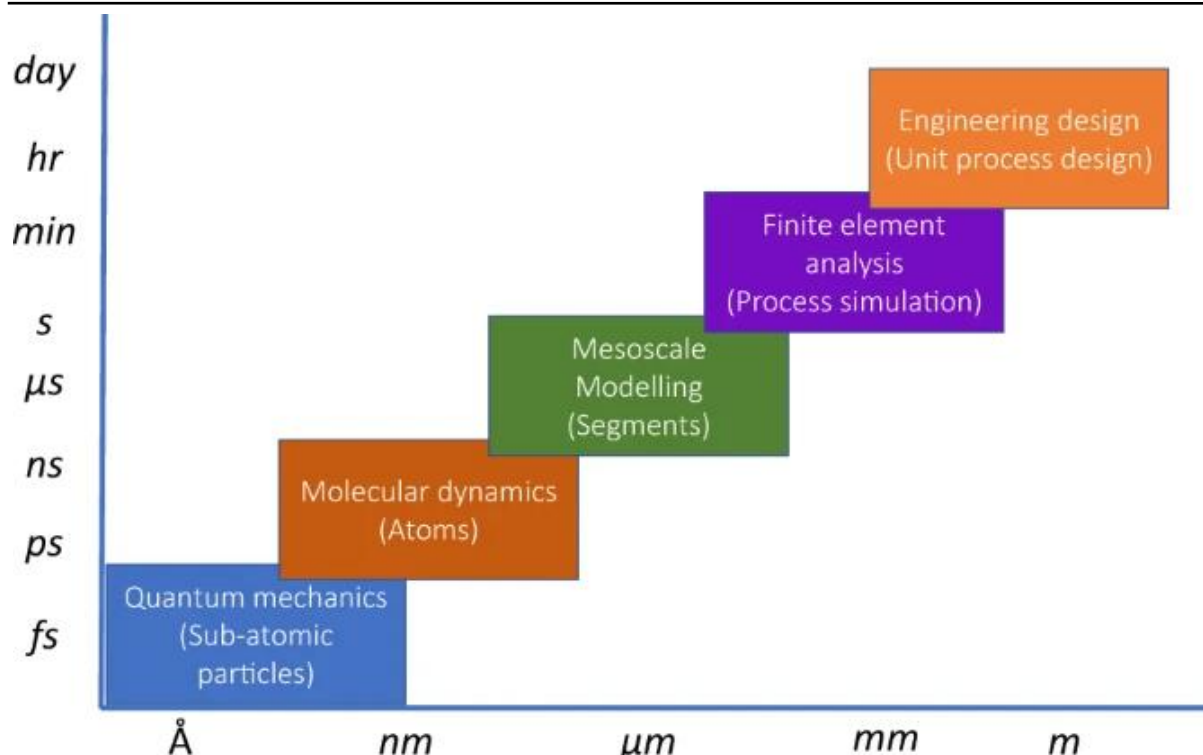


Figure 2: Length and time-scale based computational materials design techniques [22].

Applications of DFT in Materials

Density Functional Theory (DFT) is a powerful quantum mechanical modeling tool used to predict and analyze the structural, electronic, optical, and mechanical properties of materials from an atomistic level. Primary important applications of DFT in

materials include modeling battery electrodes, designing solar cell materials, calculating band structures, predicting phase stability, analyzing adsorption processes, and evaluating material mechanical strengths like elasticity and toughness [25-26]. Applications of DFT in materials science, categorized for clarity shown in Table 2:

Table 2: Application of Density Functional Theory in Materials Sciences

Category	Applications	Specific Examples & Uses
Energy Materials	Batteries, Supercapacitors, Fuel Cells	Predicting Li/Na ion diffusion paths and barriers in cathode materials. Optimizing electrode materials for stability and capacity.
Catalysis	Heterogeneous Catalysis, Photocatalysis	Modeling surface adsorption, reaction pathways, activation energies, and active sites (e.g., CO oxidation on gold nanoparticles, water splitting on TiO ₂).
Electronic Structure	Semiconductors, 2D Materials, Quantum Dots	Calculating band structures, density of states (DOS), and bandgaps. Understanding graphene and TMDs (e.g., MoS ₂).
Mechanical Properties	Metals, Alloys, Composites, Ceramics	Predicting elastic constants, bulk modulus, tensile strength, and deformation mechanisms (e.g., in steel, aluminum).
Optical Properties	Photovoltaics, Display Tech, Sensors	Using TD-DFT to simulate excited states for absorption/emission spectra. Designing, perovskite nanocrystals, and plasmonic materials.
Environmental	Gas Capture, Pollution Control	Designing carbon-based materials for CO ₂ capture and degradation of pollutants.
Biomaterials	Drug Delivery, Implants	Designing drug delivery polymers, studying biocompatibility, and simulating corrosion resistance of implants.
Magnetic Materials	Spintronics, Permanent Magnets	Modeling magnetic structures, anisotropy, and magnetization in thin films and alloys.

Density Functional Theory for Nanomaterials

DFT simulations applied to nanomaterials, including Optimal Geometries, Band Gap and Electronic Properties, Density of States (DOS), Natural Bond Orbitals (NBO), and spectroscopic features (Infrared, Raman Spectra, and UV-Visible Spectra) [27-28]. Modern density functional theory (MDFT), which is based on first principles, is capable of predicting material properties and has now become

an indispensable modeling toolbox of scientists in myriad fields [29]. DFT calculates total energy based on electron density, making it essential for predicting atomic-scale properties of 0D, 1D, and 2D nanomaterials. Density Functional Theory simulations applied to nanomaterials and nanomaterials properties shown in Figure 3.

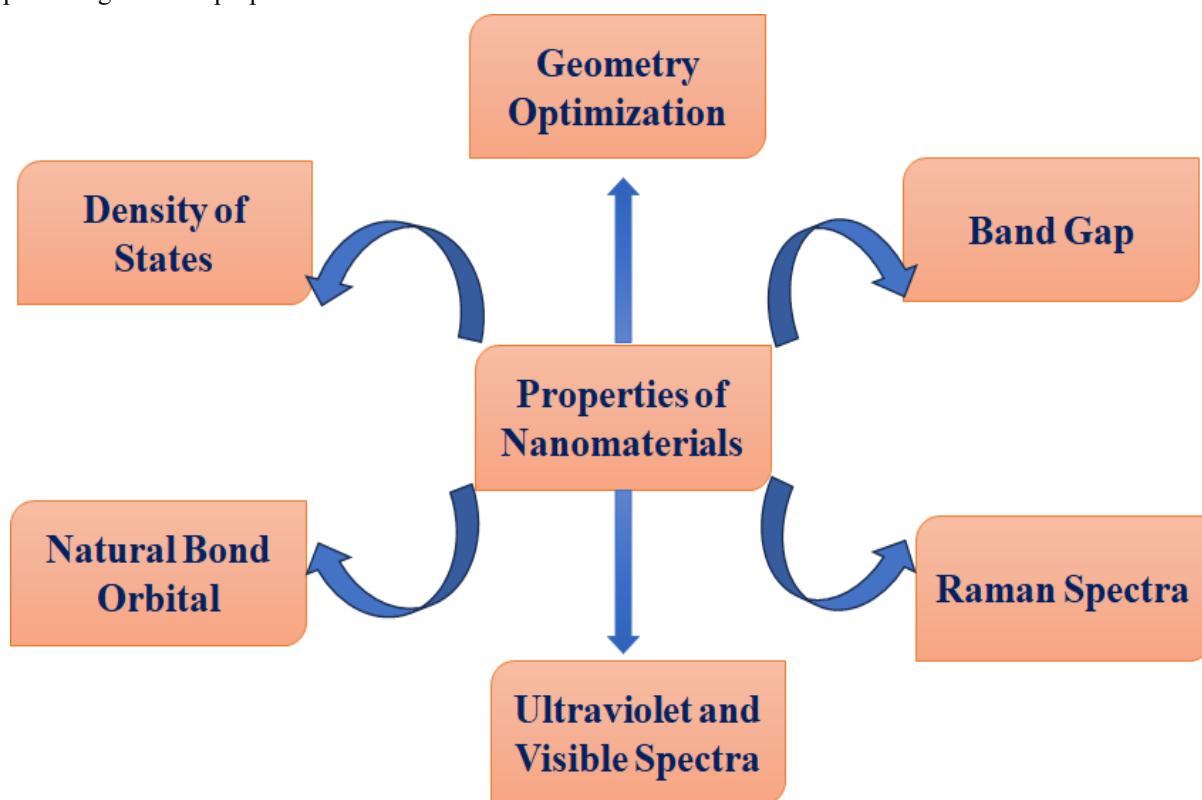


Figure 3: Density Functional Theory simulations applied to nanomaterials and nanomaterials properties

Applications of Density Functional Theory for Nanomaterials

Density Functional Theory (DFT) is now one of the important tools for studying and predicting the characteristics of nanomaterials [30]. Another way to say DFT is a powerful, first-principles computational method used to model the structural, electronic, optical, and magnetic properties of nanomaterials. Applications of DFT range from the study of bulk metals and surfaces to the study of metallic nanoparticles, which is a rapidly growing area of research due to its technological relevance [31-36].

- i. **Nanoparticle Engineering:** Designing and optimizing the stability of functionalized gold nanoparticles.
- ii. **Catalysis:** Understanding surface reactions and identifying active sites on nanocatalysts.

- iii. **Optoelectronics:** Modeling the behavior of quantum dots and thin films.
- iv. **Gas Sensors:** Predicts the interaction between gas molecules and nanomaterials, including binding energy, charge transfer, and sensor recovery times.
- v. **Bio-imaging and Drug Delivery:** Models nanoparticle interactions with biological environments and assists in designing targeted drug delivery systems.

Opportunities and Future Directions

CONCLUSION

In this review article, we have discussed the importance of DFT calculations, nanodevices applications, and nanoparticles properties for understanding and predicting key properties of

nanostructured materials. The author highlights how the combination of density functional theory, theoretical background and fundamentals, hybrid fundamentals of DFT, and classification of selected functional materials with respect to the mechanism has invigorated research in nanomaterials. The author discussed how DFT has been widely used to understand the classification of selected functional materials with respect to the Mechanism, time-scale

based computational materials design techniques, simulations applied to nanomaterials, and nanomaterial properties of various types of nanomaterials. Clearly, DFT calculations have an important role in this field, being able to describe nanoscience engineering, gas sensor, optoelectronics, drug delivery, nanomaterials, structural and electronic properties.

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