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Fundamentals of Density Functional Theory: Recent Developments, Challenges and Future Horizons

Muhammad Aamir Iqbal, Naila Ashraf, Wajeehah Shahid,
Deeba Afzal, Faryal Idrees and Raice Ahmad

Abstract

Density Functional Theory (DFT) is a powerful and commonly employed quantum mechanical tool for investigating various aspects of matter. The research in this field ranges from the development of novel analytical approaches focused on the design of precise exchange-correlation functionals to the use of this technique to predict the molecular and electronic configuration of atoms, molecules, complexes, and solids in both gas and solution phases. The history to DFT's success is the quest for the exchange-correlation functional, which utilizes density to represent advanced many-body phenomena inside one element formalism. If a precise exchange-correlation functional is applied, it may correctly describe the quantum nature of matter. The estimated character of the exchange-correlation functional is the basis for DFT implementation success or failure. Hohenberg-Kohn established that every characteristic of a system in ground state is a unique functional of its density, laying the foundation for DFT, which is being utilized to explore the novelty of materials. This chapter is aimed to present an overview of DFT by explaining the theoretical background, commonly used approximations as well as their recent developments and challenges faced along-with new horizons.

Keywords: DFT, Kohn-Sham equations, exchange-correlation functionals, challenges

1. Introduction

Density functional theory (DFT) is a low-cost, time-saving quantum mechanical (QM) theory, used to compute many physical characteristics of solids with high precision. The research in this field ranges from the development of novel analytical approaches focused on the design of precise exchange-correlation functionals to the use of this technique to predict the molecular and electronic configuration of atoms, molecules, complexes, and solids in both gas and solution phases. The history to DFT's success is the quest for the exchange-correlation functional, which utilizes density to represent advanced many-body phenomena inside one element formalism. If a precise exchange-correlation functional is applied, it may correctly

describe the quantum nature of matter. The estimated character of the exchange-correlation functional is the basis for DFT implementation success or failure. DFT's early breakthroughs concentrated on the most fundamental issues in chemistry, such as the opportunity to generate functionals that could describe both molecular geometries as well as dissociation energy. The fact that every feature of a system in ground state is a unique ground state density functional was demonstrated by Hohenberg-Kohn, laying the foundation for DFT, which is now used to explore novelty of materials. This chapter is aimed to present an overview of DFT by describing the theoretical foundations, widely used approximations, current advances, and issues addressed, as well as future horizons.

2. Fundamentals of DFT

The Schrodinger Equation [1] for a many body system may be simplified to Kohn-Sham equation, which is a single particle independent Schrodinger equation, and can be numerically solved with density functional theory. This computational process produces physical characteristics of solids; however, this hypothesis is based on electron density rather than wave functions, for which scientist Walter Kohn was given the Nobel Prize in 1998 [2]. Despite the fact that no exchange-correlation effects had been documented at the time, Thomas and Fermi claimed in 1927 that total density is the essential parameter in many body problems [3, 4]. The theorems of Hohenberg, Kohn, and Sham laid the groundwork for DFT in 1964, stating that the functional of a many-body problem's (non-degenerated) ground state electron charge density may completely characterize all properties in absence of magnetic field [5].

2.1 The Hohenberg - Kohn (HK) theorems

Hohenberg and Kohn [6] stated seemingly two simple theorems in 1964 that enabled the implementation of DFT.

Theorem I: The external potential, $V_{ext}\left(\vec{r}\right)$ is a unique functional of electron density $\rho(\vec{r})$, having a unique association among potential and electron density for a many body system; $V_{ext}(\vec{r}) \implies \rho(\vec{r})$, whereas this electron density can be used to describe the entire information of the system.

In order to establish a mathematical relation, let us assume external potentials as $v(r)$ and $v(r')$, whereas the change between these potentials is always identical since the ground state electron density is comparable at entire parts of the crystal, that is, $v(r') - v(r)$ = constant. According to theory, electrons move in a field produced by external potential V_{ext} and interact with one-another in addition to their external potential, and the corresponding Hamiltonian of energy can be written as;

$$H = T + V_{ext} + U \tag{1}$$

Where T, U, and V_{ext} represents the K.E of electrons, coulomb interaction, and external potential respectively. Quantum mechanically the factors T, U, and V_{ext} can be expressed as;

$$T = \frac{1}{2}\int[\nabla\psi^*(r)\nabla\psi(r)]dr \tag{2}$$

$$V = \int[v(r)\psi^*(r)\psi(r)]dr \tag{3}$$

$$U = \frac{1}{2} \int \left[\psi^*(r') \psi^*(r) \psi(r') \psi(r) \frac{1}{|r-r'|} \right] dr dr' \tag{4}$$

The solution of Hamiltonian for Eq. (1) can be expressed as;

$$H\psi(r_1, r_2, \ldots \ldots \ldots r_N) = E\psi(r_1, r_2, \ldots \ldots \ldots r_N) \tag{5}$$

The $\psi(r_1, r_2, \ldots \ldots \ldots r_N)$ is a ground state N interacting particle's wave-function. Suppose an additional potential $v'(r)$ with changed Hamiltonian H' and wave-function $\psi'(r)$ where the ground state density $\rho(r)$ must remain the same for both cases. The Hamiltonian for this many-body system can be written as; $H'\psi' = E'\psi'$.

Following a thorough exploration of the situation, established on $v(r)\text{-}v(r') = $ constant, it can be concluded, that $\psi(r)$ and $\psi'(r)$ are different; as a result, they both fulfill distinct Schrodinger wave equations. According to variational principle, it is an irrefutable reality that no wave function may produce energy lower than that of the ground stateψ (r) and this fact can be characterized as $\langle\psi|H|\psi\rangle < \langle\psi'|H|\psi'\rangle$ where $E = \langle\psi|H|\psi\rangle$.

Employing essential property of ground state:

$$\langle\psi'|H|\psi'\rangle = \langle\psi'|H'|\psi'\rangle + \int \left[v\left(\vec{r}\right)\text{-}v'\left(\vec{r}\right) \right] \rho\left(\vec{r}\right) dr \tag{6}$$

Alternatively, by swapping;

$$\langle\psi|H'|\psi\rangle = \langle\psi|H|\psi\rangle + \int \left[v'\left(\vec{r}\right)\text{-}v\left(\vec{r}\right) \right] \rho\left(\vec{r}\right) dr \tag{7}$$

By adding above equations we get;

$$E + E' < E' + E \tag{8}$$

The Eq. (8) confirms clear disagreement, and two unlike potentials, $v(r)$ as well as $v'(r)$ will certainly provide different density $\rho(r)$ and $\rho'(r)$ respectively. As a result, details relating density and external potential are needed to determine the Hamiltonian information. Also, T and U are known for N-partials systems so $\rho\left(\vec{r}\right)$ may be employed to find ground state H and E. The functional association of minimum energy state and corresponding resulting density is;

$$E[\rho(r)] = T[\rho(r) + V[\rho(r)] + U[\rho(r)] \tag{9}$$

Theorem II: The true ground state density of an electron corresponds to electron density that minimizes the overall energy of the functional.

Consider, $\rho(r)$ is the density which corresponds to ground state while $\rho'(r)$ to any other state of a many-body system. The functional for total energy in this context is given as; $E[\rho'] > E[\rho]$. Also, assume that $F[\rho(r)]$ is a general functional that is valid for fixed electrons at all external potentials. Mathematically this can be written as;

$$F\rho(r)] = T[\rho(r)] + U[\rho(r)] \tag{10}$$

Also,

$$E[\rho(r)] = \int [v(r)\rho(r)] dr + F[\rho(r) \tag{11}$$

In order to have minimum energy functional, the corresponding density $\rho(r)$ must be essentially a ground state density.

$$E[\psi'] = (\psi', V\psi') + (\psi', T + U)\psi' \tag{12}$$

Assuming ψ is ground state function associated to $\rho(r)$ for external potential $v(r)$, the $\rho'(r)$ will correspond to higher energy in accordance with the variational principle.

$$E[\psi'] = \int [v(r)\rho'(r)]dr + F[\rho'(r)] > E[\psi] = [v(r)\rho(r)]dr + F[\rho(r)] \tag{13}$$

As a result, provided the density functional is accurately described, one may easily compute the ground state density as well as energy in an identified external potential. Furthermore, it also demonstrates that $\rho(r)$ minimize the energy functional $E[\rho(r)]$.

2.2 The Kohn-Sham (KH) equations

The theorems given by Hohenberg-Kohn are exact; however not very useful in real calculations [6]. The equation given by Kohn-Sham [7] turned DFT into an applied tool. They converted the difficult problem of electrons interacting together in external effective potential (V_{ext}) into the electrons that are non-interacting in V_{ext}, and the total energy for a ground state of interacting electrons in fixed potential, $v(r)$ is;

$$E[\rho(r)] = V[\rho] + U[\rho] + G[\rho] \tag{14}$$

Where universal density functional $G[\rho]$ holds exchange-correlation, and is expressed as;

$$G[\rho(r)] = T_s[\rho] + E_{xc}[\rho] \tag{15}$$

$$E[\rho(r)] = T_s[\rho] + V[\rho] + U[\rho] + E_{xc}[\rho] \tag{16}$$

The kinetic energy for a many body system having non-interacting electrons is denoted by $T_s[\rho]$, while $V[\rho]$ is the external potential produced by core having positive charge, $U[\rho]$ is coulomb potential as a result of electron–electron interactions, and $E_{xc}[\rho]$ is the energy due to exchange-correlation effects.

$$T_s[\rho(r)] = -\frac{\hbar^2}{2m}\sum_i^N \int \varphi_i^*(r)\nabla^2\varphi_i(r)d^3r = T\left[\varphi_i\sum(\rho)\right] \tag{17}$$

and

$$U[\rho] = \frac{q^2}{2}\int \left[\frac{\rho(r)\rho(r')}{|r-r'|}\right]drdr' \tag{18}$$

$$V[\rho] = \int v(r)\rho(r)dr \tag{19}$$

The exchange correlation energy $E_{xc}[\rho]$ for a many-body system produced by $\rho(r)$ is given by;

$$E_{xc}[\rho] = \int [\rho(r)\varepsilon_{xc}\rho(r)]dr \qquad (20)$$

and

$$E_{xc}[\rho] = E_x[\rho]_{exchange} + E_c[\rho]_{correlation} \qquad (21)$$

The E_x term denotes the reduction in energy as an outcome of anti-symmetrization, and it may be represented through a single particle orbital as;

$$E_x = \int [\rho(r)\varepsilon_x\rho(r)]dr \qquad (22)$$

and

$$E_c = \int [\rho(r)\varepsilon_c\rho(r)]dr \qquad (23)$$

and

$$\varepsilon_x[\varphi_i\rho(r)] = \frac{-q^2}{r}\sum_{j,k}\int d^3r'(r)\varphi_k^*(r)\frac{\varphi_j^*(r')\varphi_k^*(r')\varphi_k(r)}{|r\text{-}r'|} \qquad (24)$$

Where the single term in the summation refers to the energy of a molecule 'j' at site 'r' in relation to a molecule 'k' at 'r''. The system's energy is further reduced owing to mutual avoidance of the interacting particles, such as electrons that are anti-parallel and lower their energy by evenly arranging their moments. Kohn-Sham mapping of interacting and non-interacting system is shown in **Figure 1**.

$$\varepsilon_c = \sum_{j<k}\frac{q^2}{|r\text{-}r'|} = \frac{q^2}{2}\int d^3r\int\left[\frac{\rho(r)\rho(r')\text{-}\rho(r)\delta(r\text{-}r')}{|r\text{-}r'|}\right]d^3r' \qquad (25)$$

The energy of ground state may be obtained by differentiating Eq. (14) with respect to $\rho(r)$

$$0 = \frac{\delta E[\rho]}{\delta\rho(r)} = \frac{\delta T_s[\rho]}{\delta\rho(r)} + \frac{\delta U[\rho]}{\delta\rho(r)} + \frac{\delta V[\rho]}{\delta\rho(r)} + \frac{\delta E_{xc}[\rho]}{\delta\rho(r)} = \frac{\delta T_s[\rho]}{\delta\rho(r)} + v(r) + V_c(r) + E_{xc}(r) \qquad (26)$$

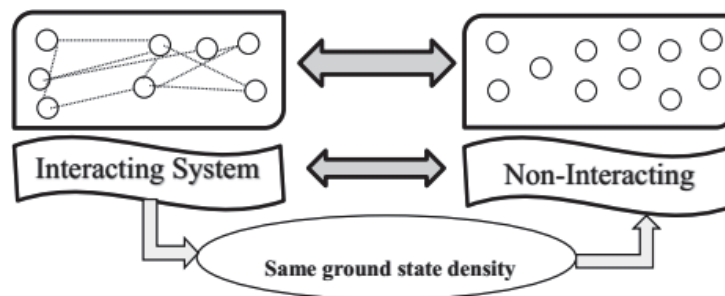By employing density $\rho_s(r)$, the minimum state for a non-interacting many-body system is;

Figure 1.
Kohn-Sham mapping of interacting and non-interacting system.

$$0 = \frac{\delta E_s[\rho]}{\delta \rho_s(r)} = \frac{\delta T_s[\rho]}{\delta \rho_s(r)} + \frac{\delta V_s[\rho]}{\delta \rho_s(r)} + \frac{\delta V_s[\rho]}{\delta \rho_s(r)} = \frac{\delta T_s[\rho]}{\delta \rho_s(r)} + v_s(r) \qquad (27)$$

Equating Eqs. (26) and (27), the potential V_s can be obtained as;

$$v_s = V(r) + V_c(r) + V_{xc}(r) \qquad (28)$$

The equation for a one-particle system that is non-interacting in potential $v_s(r)$ can be derived from the equation of interacting electrons of the system in the presence of $v(r)$.

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + v_s(r) \right] \varphi_k(r) = E_k \varphi_k(r) \qquad (29)$$

The $\rho(r)$ of an original system is replicated by orbitals, where f_k is the kth orbital occupation, and can be expressed as;

$$\rho(r) = \rho_s(r) = \sum_k^N f|\varphi_k(r)|^2 \qquad (30)$$

2.3 Exchange-correlation potential

The consequences of KS scheme revealed that the minimum energy state can be established by limiting energy of the energy functional, and it can be done using an agreeable solution of a set of single-particle equations. In the KS scheme, just one critical difficulty is that E_{xc} (exchange-correlation energy) cannot be found exactly. If E_{xc} is determined accurately, it is a precise solution for a many-body problem. There is currently no such exact solution exists, hence approximations are employed to estimate E_{xc} with LDA and GGA being the most commonly used approximations.

3. Commonly used exchange-correlation approximations

In this part, we will go through some of the major advances that lead to contemporary DFT in order to lay a foundation that will help us to comprehend both the theory's foundations and limits. Bloch (1929) was the first to write about the exchange contribution, and it has become well-known as a result of quantum Monte-Carlo simulations of uniform gases [8], which are parameterized in simple formulations [9, 10]. The Local Density Approximation (LDA) [11], proposed by Kohn and Sham, asserts that the exchange-correlation functional at any point in space is simply dependent on that location's spin density. LDA is quite correct for geometries, but it often over-binds atoms/molecules roughly by 1 eV per bond, rendering it ineffective for thermo-chemistry [12]. The Generalized Gradient Approximation (GGA) [13, 14] is an extension to the LDA component that includes terms that are dependent on density derivatives. Perdew was the first to apply real-space cutoffs to make GGAs, which led to the development of the PW86 functional model [13]. The PW91 functional [15] was the pinnacle of this comprehensive development, and it produces useful precision for binding energies, as proven in 1993 of around 6–10 kcal/mol [16]. PBE [17] is the most widely used GGA to investigate materials today, whereas BLYP [18] and Lee-Yang-Parr correlation [19] is the most generally employed GGA in chemistry. A hybrid GGA [20] is one that combines a normal GGA plus a Hartree-Fock component, in which the kinetic energy density is also employed to define the

GGA component. The GGA, Hartree-Fock, and kinetic energy density components are all present in a meta-hybrid, while hybrid or meta-hybrid component of a double-hybrid includes an involvement from second-order Moller-Plesset perturbation theory [21]. The Density Functional (DF) consists of a part of GGA, LDA, Hartree-Fock exchange or hybrids, and/or a meta-GGA, commonly known as the exchange-and-correlation (XC) functional (meta-GGA or meta-hybrid). Furthermore, the addition of an orbital-dependent correlation, it may also be reliant on virtual Kohn-Sham orbitals (double-hybrids) [22]. A comparison of simplicity versus accuracy of existing approximations in DFT is shown in **Figure 2**.

The functionals currently utilized in DFT simulations constitute a natural hierarchy, and no systematic approach to the precise functional can be claimed. The available functional form is clearly improving, resulting in a considerably more accurate representation of ground state properties. The most important recent advancements are those that include the non-local aspect of the exchange potential in some way. **Table 1**, summarizes the present hierarchy.
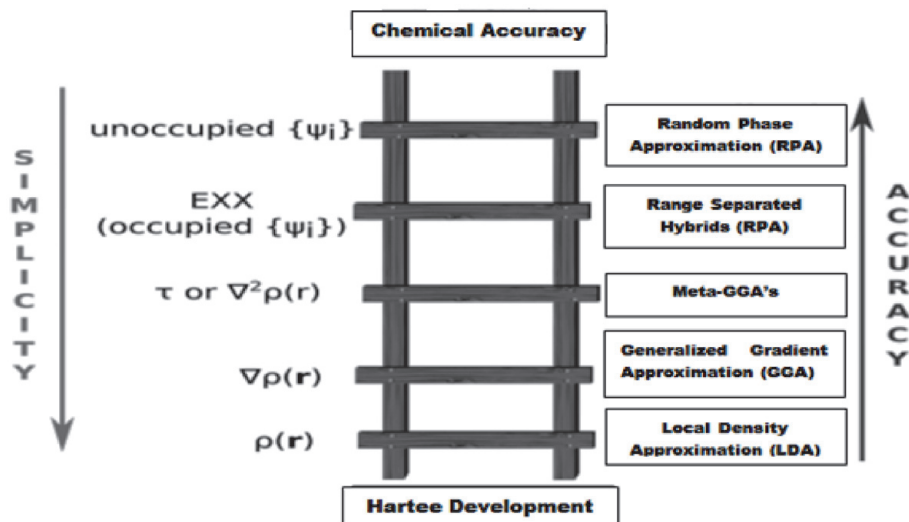

Figure 2.
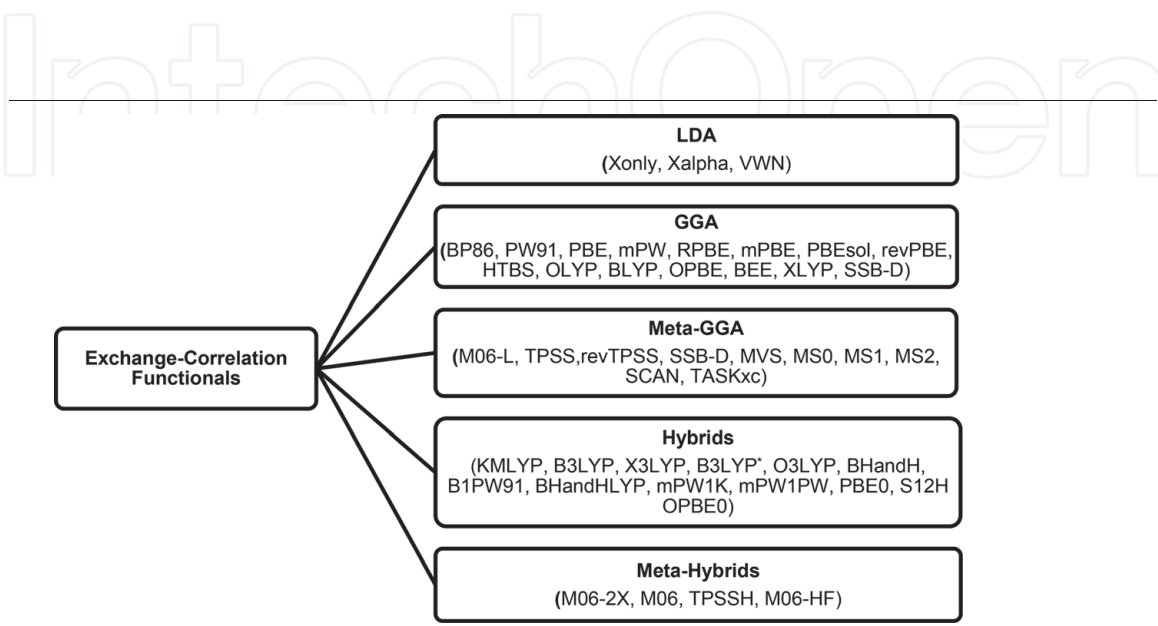*A comparison of simplicity versus accuracy of existing approximations in DFT [23].*

Table 1.
Commonly used E_{xc} functionals.

4. Recent developments

This section focuses on the evolution of new functionals in DFT during the last decades.

4.1 Random phase approximation (RPA-type Functionals)

The exchange correlation energy (E_{xc}) can be calculated using DFT fluctuation dissipation in the form of coupling constant and frequency [24–26]. The direct random-phase approximation (RPA) [27, 28] or time dependent TD-Hartree, are the results of ignoring the exchange kernel of TDFT. A fifth-rung approximation is generated as a result of this methodology, and this can be expensive to examine, although the relative burden is always reducing [29, 30]. It only examines bubble diagrams in the many-body expansion of the energy, so direct RPA over-correlates systems by ignoring extra contributions at higher levels that diminish correlation. It also has issues with self-interaction since, even when just one electron is involved, it yields low correlation energies, and the dissociation energies of molecules are erroneous [23].

4.2 Meta-GGA's

The meta-GGA [31] is a novel component that extends beyond density and gradient, and is commonly used to indicate the KS orbitals' kinetic energy density. The objective of a successful meta-GGA is to achieve hybrid accuracy without incurring the computational expense of the exact exchange contribution. The incorporation of atom-centered basis functions, the cost of accurate exchange is reasonable, however, it can be costly while using periodic boundary conditions in addition of basis sets. Perdew and colleagues, and plenty of others, have worked on meta-GGAs for decades, with multiple failed attempts [32]. SCAN (strongly constrained and suitably normed semi-local density functional) [33], the most current effort has undergone a number of conventional tests and looks to have a good chance of becoming part of the pantheon of widely employed functionals. The G3 data-set [34] is a common collection of chemical compounds that LDA over-binds around 3 eV, while PBE reduces it to approximately 1 eV, and SCAN around 1/4 eV. On the S22 data-set [35] of weakly bonded systems, SCAN has 2–3 times less errors than PBE does, while SCAN decreases miscalculations of lattice constant and other parameters on the LC20 data [36] set around 0.05 Å, and to around 0.01 Å in PBE. The PBE [37], on contrary to SCAN, only improves underestimation of chemical barrier height by 30 percent, while hybrids on the other hand are frequently 2–3 times superior with conventional varieties. Therefore, one can conclude that SCAN achieves accuracies comparable to hybrid functionals for several characteristics at a fraction of the computing cost [38].

4.3 Range separated hybrids (RSH)

Andreas Savin was the first to create the range separation hypothesis, which is quite precise [39, 40], through which coulomb repulsion may be easily expressed by combining a short-ranged input with a long-ranged involvement that do not have coulomb singularity at zero separation, and decays quicker than the inverse of the separating distance. In KS equation generalizations, one contribution is treated as an interaction, while the other is compensated by a redefined XC contribution. The HSE06 functional [41] is a hybrid with a range separation that manages long-ranged

exchanges with an approximation, short-ranged exchanges with accuracy in an extended insulator [42], and this combination frequently yields exact gaps for moderate-gap semiconductors and insulators [37].

4.4 Weak interactions

Over the last two decades, tremendous progress has been made in addressing the challenges associated with weak van der Waals (vdW) interactions. Traditional functionals do a good job at manipulation of covalent, ionic, and metallic interactions due to their semi-local nature, but they fall short when it comes to longer, weaker bonds, and cannot offer weak binding that drops off as a function of R^6 (R is the distance among two atoms) [38]. To account these impacts, modifications must be applied to the conventional functionals and this can be accomplished in one of three ways. There is a succession of approximations produced by Langreth and Lundqvist and collaborators [43] for the evolution of explicit non-local functionals of electron density, while these approximations are generated non-empirically, notably beginning with contributions of correlation energy. Additionally, these functionals may be useful for any materials, ranging from solids to molecules, and have been designed by supposing systems that contain a gap [44]. RPA, which incorporates approximations to the vdW forces by default, as well as the Becke and Johnson technique [45], leverages the exchange hole's dipole moment to approximate C_6, as well as higher coefficients.

4.5 Gaps of solids

The inadequacy of traditional approximations to anticipate band gaps of semiconductors and insulators is a critical flaw. The LDA undervalues gap between bulk Si and Ge by a factor of two, making Germanium a metal, whereas GGAs performs a bit good but underestimate as well. The ability to give precise and dependable gaps has always been a strong suit of the GW approach [46]. In the last two decades, precise gap computation utilizing hybrid functionals such as HSE06 [41] has been a huge success, and is accomplished through the use of a generalized KS scheme [47]. In this case, rather than using pure Kohn-Sham theory, the orbital reliant element of the functional is considered as in Hartree-Fork approach to overcome flaws of other E_{xc} functionals [48].

5. Challenges for DFT

In principle, DFT is exact; however its effectiveness depends on the development as well as advancement in exchange-correlation (E_{xc}) functionals which may be achieved by optimizing against larger data-sets and using improved functional arrangements that are more flexible and contain more elements. Smoothness has also been prioritized in recent enhancements, which helps to alleviate problems like grid-size convergence and self-consistent field iterations. In this section, we will go through some of DFT's challenges that may differ from those that appears to be "solved" to those that are still being explored. There are numerous more that are less well-known, and yet crucial to DFT's future growth as well as use.

5.1 Strong correlation

DFT's inadequacy for strongly correlated systems utilizing typical approximations has been acknowledged since its inception, and this can be investigated as well

as linked to standard approximation localization or delocalization inaccuracies when integer or half-integer electron quantities are found in distinct locations [49]. In quantum computational physics and chemistry, the Kohn-Sham gap among two states becomes too narrow, and the wave function of a many-body system is very nearly equal to mixing of two slater determinants, which is referred to as static correlation. The failure of approximations under these situations cause the challenges, not the KS scheme itself, as demonstrated by the two-site Hubbard model, in which the precise KS system is simple to design, even when one deal with strongly correlated systems [50]. This problem can be addressed by breaking the symmetry of evenly spaced atomic chains into multiple solutions, and one of which will have the least amount of energy [51]. This is such a significant issue; hence, a great deal of research has been done on it, particularly by Weitao Yang's group [52], but also by Scuseria [53] and Becke [54].

5.2 Development of uniformly better and simple functionals

One of the biggest problems for DFT is to preserve some aspect of simplicity as its foundations. When DFT functionals get as complicated as full configuration interaction, one of the theory's most significant properties, namely simplicity, is lost, which is particularly true in terms of computational environment. This simplicity, however, must not be at the expense of accuracy, nor should it become an exclusively empirical approach. The precise representation of binding energies and geometries of simple molecules was one of DFT's first major hurdles in chemistry. Becke, Perdew, Langreth, and Parr presented the density's first derivative in the form of generalized gradient approximation in the 1980s, which was the first step towards chemists being able to correctly use DFT. In the early 1990s, Becke described the proportion of Hartree-Fock exact exchange (HF) which is included in the functionals, and as a result of this effort, B3LYP [55], the utmost extensively utilized of all the functionals, was developed, and has demonstrated outstanding performance in variety of systems. Despite the introduction of new concepts into more current functionals of varying complication, it remains the prevalent, and DFT will likely benefit from developing functionals that improves on B3LYP [56].

5.3 Dispersion and reaction barriers

To provide a comprehensive chemistry explanation, it is indispensable to go beyond explaining a molecule in equilibrium geometry to similarly explain weakly interacting atoms or molecules, and chemical reaction transition states. It's challenging to describe reaction barriers with LDA or GGA functional since they consistently underestimate the difficulty of transitioning from one condition to another. Formerly the functionals may be utilized to represent potential energy surfaces, and this systematic imperfection must be corrected. Transition states, covalent bonding, and van der Waals attraction are all challenging to represent precisely and effectively, though efforts are to be made to address these problems. This is especially true when DFT becomes more widely applied to biologically important regions, where all of these interactions might occur at the same time [57].

5.4 Static correlation and delocalization errors

The enactment of DFT, as evidenced by significant errors for one-electron systems, is another important issue. In DFT, a single electron system has no exceptional role; in fact, one electron can interrelate with itself, as the self-interaction error has long proved. Of course, there is no self-interaction in the accurate
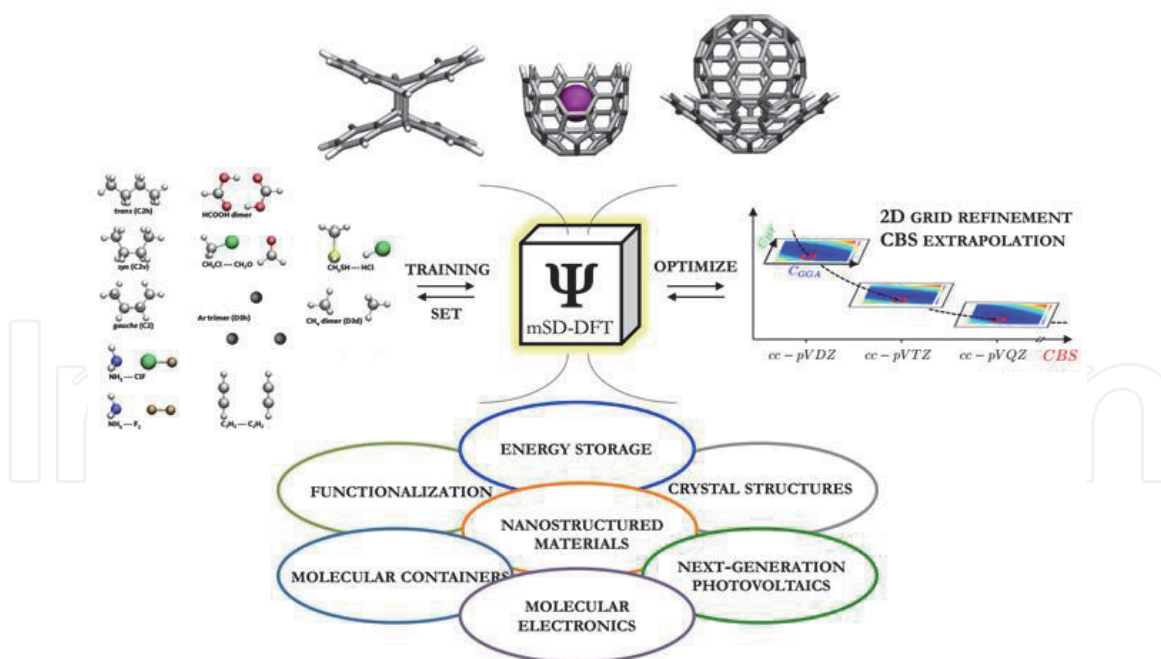
Figure 3.
Potential application areas of DFT [61].

functional; the exchange energy precisely cancels the coulomb energy of single electron. In increasingly complicated systems, they can be linked to systematic flaws like static correlation and delocalization error, and despite most recent advancements, even the simplest systems can contain mistakes in most recent functionals [58]. Hence, these basic systems should not be overlooked since they hold the vital knowledge of functionals that can lead to advancements [57].

6. New horizons

The applications of warm dense matter vary from modeling planetary interiors to inertial confinement fusion [59], which is a completely new field for DFT, and has been exploded in the last decade, with considerable temperatures on the electronic scale of roughly 10^5 K but not to the point that the Thomas- Fermi hypothesis or classical performance takes precedence. This domain is so "new" that temperature-dependent exchange-correlation energy of a uniform gas, which is the input to thermal LDA, is just now being computed with remarkable precision [60]. **Figure 3** summarizes some of the potential application areas of DFT.

7. Concluding remarks

Density Functional Theory is a powerful and commonly employed quantum mechanical tool for investigating various aspects of matter. This field's research ranges from the development of novel analytical approaches focused on the design of precise exchange-correlation functionals to the use of this technique to predict the molecular and electronic configuration of atoms, molecules, and solids in both gas and solution phases. Designing and evolution of more efficient density functionals is a continuous endeavor since there are still challenges to be resolved, and getting all of the attributes correct at a reasonable computing cost is a quantum fantasy. The future research will focus on developing even more consistently

precise density functionals for specific applications, allowing researchers to take use of DFT's comparatively high accuracy at cheap processing cost, and the possibility of even more improvements awaits.

Author details

Muhammad Aamir Iqbal[1*], Naila Ashraf[2], Wajeehah Shahid[3], Deeba Afzal[4], Faryal Idrees[5] and Raice Ahmad[6]

1 Centre of Excellence in Solid State Physics (CSSP), University of the Punjab, Lahore, Pakistan

2 Department of Mathematics, Government College University (GCU), Lahore, Pakistan

3 Department of Physics, The University of Lahore (UOL), Lahore, Pakistan

4 Department of Mathematics and Statistics, The University of Lahore (UOL), Lahore, Pakistan

5 Department of Physics, University of the Punjab, Lahore, Pakistan

6 Institute of Microbiology and Molecular Genetics, University of the Punjab, Lahore, Pakistan

*Address all correspondence to: aamir.phd.cssp@pu.edu.pk

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