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Bandgap Tuning and Photocatalytic Efficiency in Doped and Composite TiO_2 Systems: Insights from Hybrid DFT and TDDFT Simulations

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Abstract: This review deliberate on the process of accomplishment of enhanced photocatalytic efficiency of doped and composite TiO_2 systems. Hybrid Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT) simulations used by the several researchers to tuning the bandgap of the material. They have highlighted the significance of TiO_2 in photocatalysis and have been highlighted its main limitation; a broad bandgap that limits the ability to absorb visible light. Some of the doping and composite methods are examined in this study, exploring the effects brought about by each method for the separation of charges, light absorption, and breaking down of pollutants. It has been found that strategic doping as well as the formation of heterojunctions can dramatically enhance the charge-carrier behavior and the photocatalytic activity. The reported experimental data confirmed the TDDFT simulation results and the computational methods are useful in predicting the absorption spectrum as well as increasing the velocities of reactions. On the whole, the review reveals the significant mechanisms of the optimization of TiO_2-based photocatalysts and suggests the supplementary development of research to address the existing problems.

Keywords: Bandgap Tuning, Photocatalysis, TiO_2, Hybrid DFT, Charge Separation

1. Introduction

Titanium dioxide (TiO_2) is the photocatalyst that has been investigated owing to its chemical stability, non-toxicity, and low costs. There are numerous areas where it is applied, such as environmental cleanup and production of renewable energy. Several uses are decontamination of pollutants, water splitting, and minimize CO_2 [1]. These applications have made TiO_2 to be an important material in the quest to find sustainable technologies. Nonetheless, TiO_2 can be used due to its inherent characteristics. The anatase form of the material has a wide bandgap of approximately 3.2 eV and the rutile form of the material has a wide bandgap of approximately 3.0 eV, meaning that it can only absorb ultraviolet (UV) light [2]. Approximately about 5 percent of solar rays consist of UV light implying that TiO_2 cannot be used efficiently in regular sunlight. This has necessitated the researchers to seek a means through which it can be enhanced to achieve better efficiency as a photocatalyst. Numerous approaches have been experimented with but band-gap engineering via doping and composite materials has been particularly effective [3]. Doping introduces foreign atoms into TiO_2 lattice forming new energy levels or displacing the conduction and valence bands. This decreases the bandgap and permits the substance to absorb the light of visible color. The synthesis of composite forms enables the formation of heterojunctions with other substances as TiO_2 and improve the separation of charges and enhance photocatalytic activity [4].

This review sets out to investigate the manner in which band-gap tuning, charge separation and photocatalytic performance varies in doped and composite TiO_2 systems. Based on the simulation of the hybrid density functional theory (DFT) [4] and time-dependent DFT (TDDFT), the impact of these changes on the electronic structure, light-absorbing behavior and the degradation of the pollutants pathways were anlysed and reported by many researchers. Hybrid DFT is effective to predict electronic and optical properties, whereas TDDFT brings out dynamics of excited states and charge transfer. The combination of these computational tools provide the opportunity to investigate the correlation between structural changes and photocatalytic activity in TiO_2 [5].

There are some key points that are discussed in this review. This review started by examining doping techniques, and addition of anionic and cationic dopants, including nitrogen, sulfur and iron influences the band structure and improves absorption in the visible light region. Second, we learn about TiO_2 composites, where the synergistic effects of combining TiO_2 with such material as graphene, ZnO, and g-C_3N_4 are discussed. Third, we discuss charge-carrier processes, and, in particular, the higher efficiency of charge separation and reduced recombination enhance photocatalytic processes [6]. Fourth, we apply TDDFT to model the predictions of the absorption spectra of modified TiO_2 and other predictions using it to compare the predictions with the experimental results to test our models. Lastly, the significance of surface chemistry and active sites in the effect on the pollutant-degradation pathways is explored, demonstrating that these factors are important catalysts of photocatalysts reactions [7].

Further, this review examines some of the basic principles on which the photocatalytic behavior of doped and composite TiO_2 is based. Figure 1 outlines of TiO2 nanoparicles photocatalyst and its limitations. The results can assist researchers to develop new group photocatalysts which are efficient and effective. The following reports also consider these factors methodically, beginning with a summary of band-gap engineering in TiO_2 and the measures to enhance its photocatalytic capabilities. TiO_x is significant in photocatalysis due to the fact that it can use light and induce a chemical reaction. This makes it a multifunctional substance in improving the air and water purification, hydrogen production, and CO_2 reduction [8]. As an example, TiO_2 photocatalysts are capable of treating a wide variety of organic contaminants: dyes, pesticides, pharmaceuticals, etc. This skill is essential for addressing environmental issues such as water contamination and bad air quality. Furthermore, TiO_2 finds some applications in energy conversion, such as the water splitting and CO_2 reduction, which attracts the interest of renewable-energy scientists [9]. Through the utilization of sun rays to create hydrogen or transform CO_2 into beneficial chemicals, TiO2 photocatalysts offer a sustainable solution to the issue of energy crises and climate change across the glope. The possible and versatile nature of TiO_2 has attracted research attention in photocatalysis and materials science. Nevertheless, the implementation of TiO_2 on a large scale is restricted by its disadvantages. Its large bandgap restricts light absorption to the UV, reducing its efficiency at sunshine. The recombination rate of photogenerated electron-hole pairs is also rapid in pure TiO_2, leading to decreased availability of charge carriers to reaction. These difficulties pronounce the necessity to modify and enhance TiO_2 to achieve a practical applications using ground-breaking strategies [10].

The Schematic diagram of TiO_2 and their applications is shown in figure 2. The key problem with pure TiO_2 is that it does not utilize visible light very effectively, which accounts for approximately 45% of total solar spectrum. This is due to the fact that TiO_2 possesses large bandgap, which necessitates the high-energy UV photons, to excite them to flow out of the valence band to the conduction energy level. This means that a huge proportion of the solar energy is wasted, which reduces the photocatalytic efficiency of TiO_2 based systems [10]. The other issue is the rapid recombination of the photogenerated charge carriers. Absorption of light generates electron and hole pairs which move to the surface to produce redox reactions, however in pure TiO_2, it is common to have a rapid recombination proce

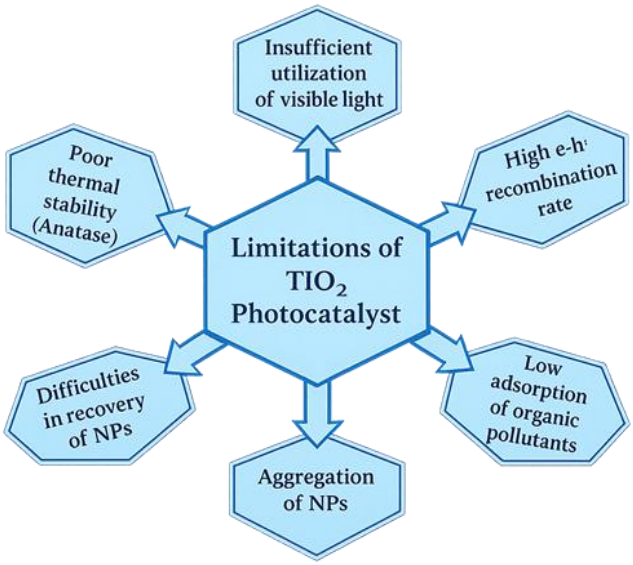

Figure 1. Outlines of TiO_2 nanoparicles photocatalyst and its limitations.

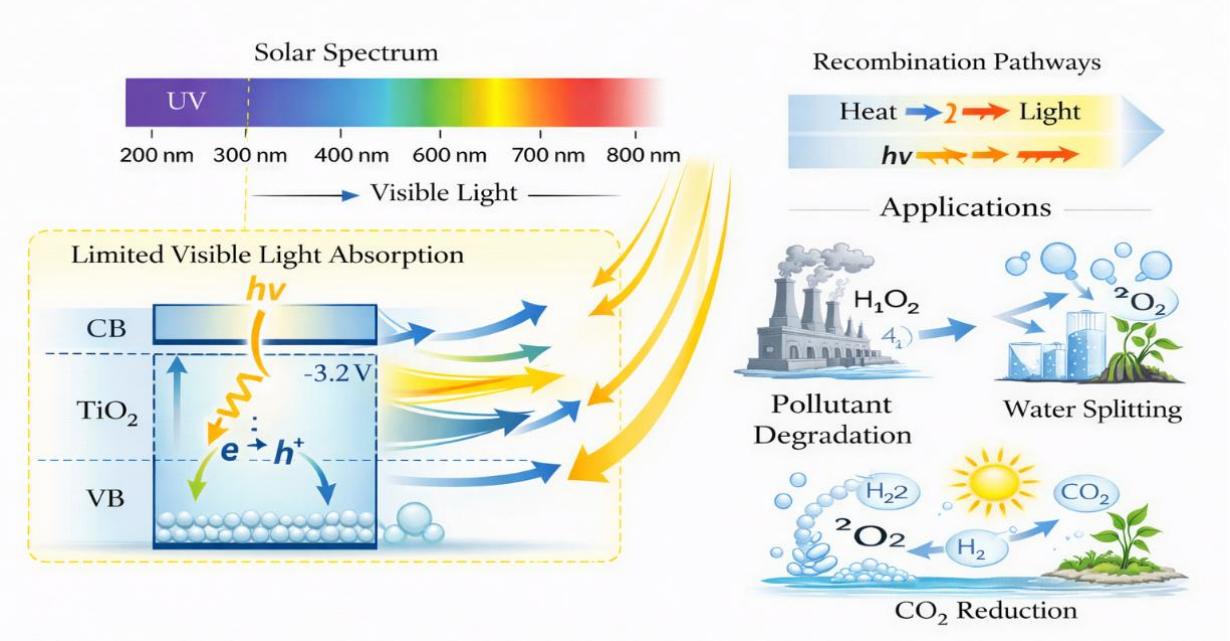

Figure 2. Schematic diagram of TiO_2 and their applications.

This is done at the expense of energy in the form of heat and overall efficiency. Thus, it is necessary to have better TiO_2 photocatalysts which are better in terms of efficiency at charge separation and longer lifetime of these carriers. To solve these problems, scientists are working on modified TiO_2 with increased ability to absorb light, charge separation and, increased photocatalytic activity. These processes can be grouped into two categories namely doping and composite formation [11].

Doping is a process that incorporates foreign atoms into the TiO_2 lattice modifying the electronic structure and optical characteristics. Anionic dopants e.g. nitrogen and sulfur produce mid-gap states that aid to absorb visible light [12, 13]. The additions of cationic impurities such as iron and tungsten cause changes in the conduction and the valence band edges, reducing the bandgap, and broadening the absorption range out to the visible spectrum. E.g. nitrogen doping introduces the localised states above the valence band to allow absorption in visible-light [14]. Optical properties can also be enhanced synergistically by co-doping with other elements, e.g. nitrogen and fluorine. The studies by hybrid DFT have raised the prospect of doped TiO_2 will in visible light driven photocatalysis. The Composite formation is a process that includes coupling TiO_2 with other materials to generate heterojunction that enhances charge separation and increase photocatalytic activity. An example is that by adding TiO_2 to graphene, the velocity of the electrons and recombination decrease. ZnO, or g-C_3N_4 composites are utilized to enhance light absorption and charge-transfer. It has been demonstrated that hybrid DFT simulations offer theoretical evidence concerning the flux to the photocatalytic properties of such TiO_2-based composites that are enhanced [14].

To conclude, pure TiO_2 has severe limitations which need modifications in order to enhance its photocatalytic ability. Through measures like doping and composite formation, scientists have gone far to overcome these problems and enhance the commercial applications of TiO_2 photocatalysts. These changes and their mechanisms will be discussed in the following sections of this paper and their effects on TiO_2 performance will be examined [15].

2. Mechanisms and Strategies of Bandgap Engineering in TiO_2

2.1 Bandgap Tuning Techniques of Doping

Titanium dioxide (TiO_2) with the use of which as a photocatalyst has been a subject of extensive research is due to its stability, no-toxicity and abundance. Photocatalysis is restricted to the ultraviolet (UV) region (approximately 3.2 eV with anatase, and 3.0 eV with rutile) of the solar spectrum, and only occupies a fraction (only a little over 5% of the solar spectrum) of the bandgap of the photocatalyst [16]. Researchers usually resort to doping to convert the activity into the visible light. In doping, anionic (non-metal) or cationic (metals) atoms are purposely introduced in the TiO_2 lattice. This will help close the bandgap, enhance visibility light absorption and enhance reaction kinetics of charge carriers to enhance the photocatalytic activity of TiO_2 [17].

Doping also modifies the electronic structure of TiO_2, either by forming impurity energy levels within the bandgap, or by altering the conduction and valence bands.

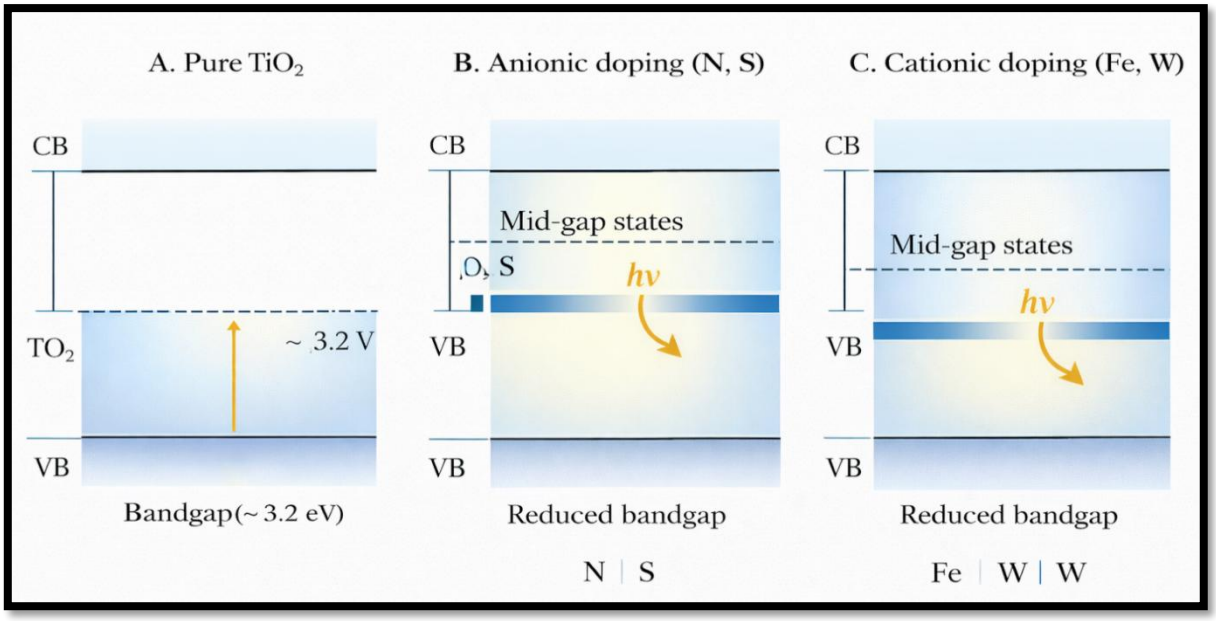

Figure 3. Bandgap Engineering of TiO_2 by doping.

Oxygen atoms in the lattice are normally substituted with the anionic dopants which include nitrogen (N) and sulfur (S) [18]. They create localized states around the valence band and reduce the energy required to make an electronic transition and facilitate absorption in the visible-light. Figure 3 displays the Bandgap Engineering of TiO_2 by doping. Sates that are more like those of a conduction band or lie inside the bandgap are added by cationic dopants such as iron (Fe) and tungsten (W), which provides changes in the dynamics of charge-carriers and lowers recombination rates [19].

Doping is effective depending on a number of factors; the ionic radius of dopant, its electronegativity, and its oxidation state. Indicatively, nitrogen has a comparable ionic radius to oxygen, which means that it readily incorporates into the lattice of TiO_2. It forms in-between states without causing a major change in the crystal structure [12]. Simulations based on the hybrid density functional theory (DFT) are used to calculate the interaction of dopants with TiO_2, providing information on electronic and optical dynamics of doped materials [20]. The research provided by Samsudin and Abd Hamid [21] proves the advantages of TiO_2 co-doping with nitrogen and fluorine (N/F). Their hybrid DFT model has shown a synergistic effect that is incredibly effective in boosting absorption in the visible and lowering the bandgap to approximately 0.95 eV. The provided example highlights the importance of sophisticated computational schemes in the design of the effective doped TiO_2 photocatalysts [22].

2.1.1 Nitrogen Doping (N-TiO_2)

One of the most widely researched anionic dopants in TiO_2 is nitrogen due to its formation of shallow acceptor states immediately above the valence band that reduces the bandgap.

The substitution of oxygen atoms with nitrogen yields N2p states which overlap with the O 2p states reducing the energy required to excite the electrons electronically [23]. As Choi *et al.* [24] demonstrated, nitrogen doping alters the TiO_2 absorption edge to the visible light. Nevertheless, too much nitrogen may form the centers of recombination that reduce the activity of photocatalysts. To balance between bandgap narrowing and charge-carrier dynamics, it is necessary to optimize the nitrogen concentration by use of hybrid DFT simulations [16].

2.1.2 Sulfur Doping (S-TiO_2)

Sulfur may be in various oxidation states, providing it with the capability to replace oxygen, as well as, fill interstitial sites in the TiO_2 lattice. Substitutional sulfur creates S 3p energies above the band of valence, whereas interstitial sulfur creates donor states around the conduction band. In a study that employed hybrid DFT simulations, Zhang and Xu [25] investigated sulfur doped TiO_2 and discovered substitutional doping to be more efficient in reducing the bandgap. The paper also demonstrated the conclusion that lattice distortion and larger surface area may also enhance photocatalytic performance, which is a multifaceted effect of sulfur doping [12].

2.1.3 Iron Doping (Fe-TiO_2)

Adding a d-state of mesenteric TiO_2 inside the bandgap of the TiO_2 transition metal serves as charge carrier traps. Such traps reduce recombination rate and increase charge separation which is essential in photocatalytic recombination. Pasang *et al.* [26] noted that iron doping reduces the bandgap in addition to increasing the density of the states around the Fermi level that enhances the light absorption and the carrier

mobility. According to hybrid DFT, when Fe concentration exceeds 2%, it may be divided into secondary phases of Fe_2O_3 that damage photocatalytic activity. A tight regulation of the doping rate is necessary [27].

2.1.4 Aluminum Doping (Al-TiO_2)

The bandgap of TiO_2 applies well with aluminum doping. Distinct redshift in the absorption edge of Al -doped TiO_2 is reported by Islam *et al.* [28, 29], and to this end the state of Al 3p in the bandgap. Experimental and theoretical evidence suggest that the bandgap narrowing enhances visible-light absorption and so, the strategy has potential in photocatalysis. Al doping also enhances the surface area and porosity of TiO_2, providing more active sites of reactions [30].

2.1.5 W-TiO_2 and Co-Doping Plans

W doping places W^{5d} states close to the conduction band to decrease the bandgap and increase absorption in the visible-light. Ullah *et al.* [28] determined that tungsten with 6% concentration nitrogen greatly enhances the Congo Red degradation. Hybrid DFT identified shallow donor states which provide transfer of charges and reduce recombination. The mid-gap states of co-doping with tungsten and nitrogen or sulfur make the continuum and increase performance, with Nair *et al.* [31] finding a significant advancement. Such synergies demonstrate how interoperative dopants can improve the shortcomings of individual dopants. Hybrid DFT techniques are a combination of Hartree-Fock exchange and DFT which is providing a better account of the electronic structure of doped TiO_2 compared to traditional DFT [12]. They measure the effects of d-electron localization and the presence of mid -gap states, essential to the study of doping effects. Hybrid DFT has been utilized to examine Ti^{3+} doped TiO_2, it was found that Ti^{3+} states in the bandgap enhance the process of light absorption and chargecarrier separation significantly. The second point that is highlighted in the studies is the manipulation of the doping environment including the use of reducing agents and alkaline environment so that optimum performance is attained. In order to study the influence of carrier concentration on the bandgap of doped TiO_2 systems, Munir *et al.* [32] applied hybrid DFT. They discovered that further addendum of dopant concentration above a critical point minimizes the bandgap and yet creates recombination centers, decreasing photo catalytic efficiency. This finding reveals the need to have accurate doping policies which put bandgap reduction and chargecarrier dynamics in a relative balance [33]. Table 1 lists the depend induced electronic structure modification. Islam and Podder [29] used hybrid DFT to study the electronic and optical properties of the TiO_2 with aluminum dopant. A good correlation was observed between calculated electronic and optical bandgap energies in their work, which justifies the computational method of predicting the behavior of doped-systems [20]. The authors emphasized the role of surface chemistry and active sites in catalyzing the photocatalytic reaction, and they demonstrated the combination of bulk and surface properties in doped TiO_2.

Table 1. Dopand induced electronic structure modification

Dopant	Mechanism	Band Effect
N	N_2p states	Valence band shift
S	S_3p states	Mid-gap states
Fe	d-orbitals	Trap states
Al	Surface states	Bandgap narrowing
W	Donor states	Conduction band shift

Doping TiO_2 anionic and cationic provides an effective method to tune the bandgap and increase the photocatalytic efficiency of TiO_2. The most active dopants are nitrogen, sulfur, iron, aluminum and tungsten, which can change the electronic structure of TiO_2 in a different manner. The sophisticated interactions of dopants with TiO_2 lattice have been deciphered by using hybrid DFT simulations and this has shed light on bandgap engineering and charge carrier dynamics. As more novel dopants and co-doping methods are being investigated, making use of both computation and experimental methods will be essential to maximize the TiO_2 based photocatalyst use in environmental clean-ups and energy generation [22].

2.1.6 Formation of Composites and Synergy

Titanium dioxide (TiO_2) is a renowned, stable chemically, non -toxic, highly oxidizing photocatalyst. Its high bandgap (3.2 eV) restricts its activities at visible light hence it is less applicable in a variety of applications. To solve this, scientists have developed TiO_2-based composite which involves the incorporation of TiO_2 and other substances to enhance photocatalytic. Composites provide combinations of superior qualities to different components, e.g., higher levels of light absorption, effective charged separation, and an elevated level of surface reactivity. Figure 4 explains the formation of composite sand synergy. As an example, the inoculation of TiO_2 to graphene, ZnO, or g-C3N4 has been suicidal but encouraging in overcoming TiO_2 shortcomings [34].

Composites utilize the exceptional properties of a secondary material to improve the photocatalysis of TiO_2. Through its high electrical conductivity and high surface area, graphene is able to accept electrons easily reducing the recombination of charges. In a similar vein, it can be noted that semiconductors such as ZnO and g-C_3N_4 may build heterojunctions with TiO_2, allowing the formation of peak secondary rates.

Such modifications enhance the total photocatalytic efficiency and expand the absorption range of light so that the visible light is utilized to a better purpose. These composites have been studied intensively by more advanced computational studies including hybrid DFT and TDDFT that provides important insights into the electronic structure and charge dynamics [35].

A design strategy of TiO_2 composites is the heterojunction formation. The interface between two compatible energy band semiconductors is the heterojunction. In the case of TiO_2 with another material, such as the graphene or the ZnO, the band alignment is used to colloquially separate the photogenerated electron-holes in space. This division decreases the recombination of charges which increases the carrier lifetime therefore increasing photocatalytic efficiency [36].

An example is TiO_2-graphene composite which has been extensively researched due to the superior electronic characteristics of graphene. Giannakopoulou *et al.* [37] synthesized and characterized TiO_2/graphene composites and observed that the charge separation efficiency improved significantly. The bandgap of the composite reduced to approximate 2.66 eV, which increased absorption with visible-light. This was enhanced by the fact that graphene had a very high electron mobility, which is a good electron sink and inhibits photogenerated electron-charge recombination [38]. Another example of common semiconductor, which has a possible heterojunction with TiO_2 was ZnO, which also shows good photochemical performance. The bandgap of ZnO (~3.2 e V) is comparable to that of TiO_2 but its bandgap is more negative which means that the electrons can be transferred out of TiO_2 to ZnO. This charge-transfer mechanism enhances the overall photocatalytic process of this composite.

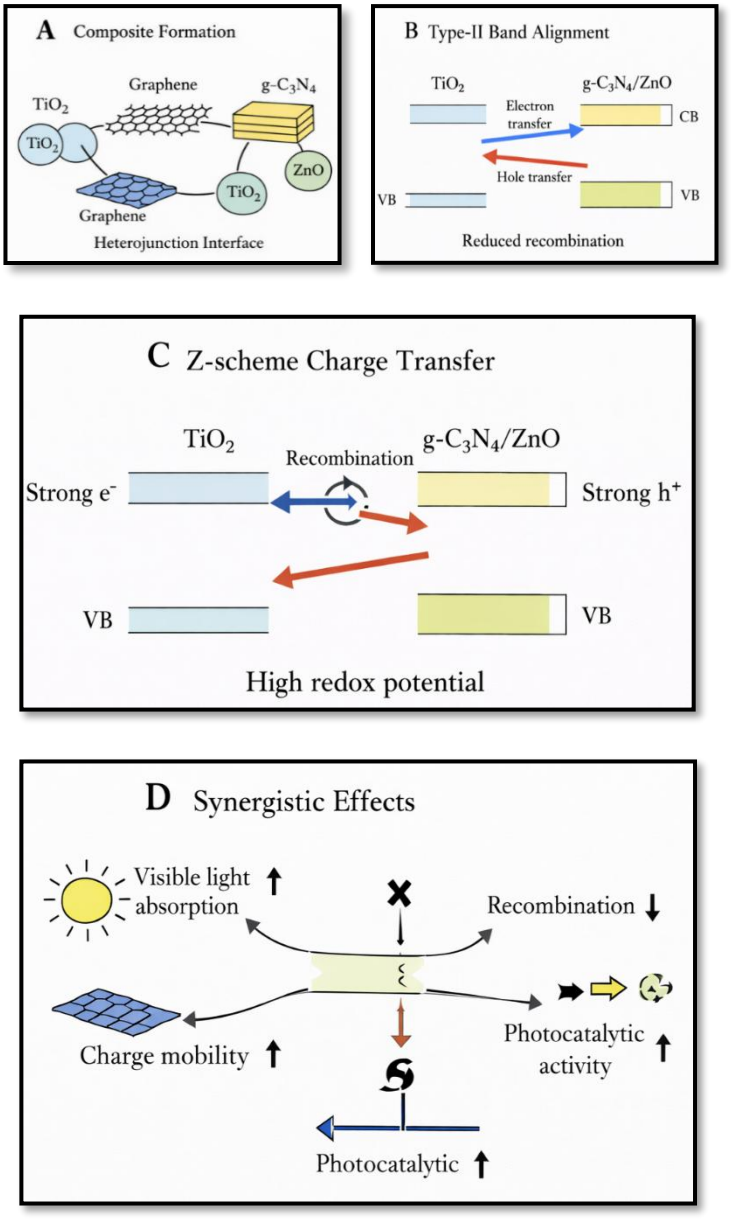

Figure 4. Formation of composite sand synergy.

Samsudin and Abd Hamid [21] focused on the ability of dopants to adapt photo-responsiveness of TiO_2/ZnO composites, in which the band-gap engineering principle underpins the need to enhance light harvesting efficiency [39]. Polymeric semiconductor g-C_3N_4, having a bandgap of approximately 2.7 eV, has itself been considered, as well as with viral nanoparticles, as a visible light absorber. Nagaraj *et al.* [40] have cited TiO_2/g-C_3N_4 composites, in which the two of them complemented the light capture and charge separation. They discovered the optical bandgap tuned to 3.09eV in the composite permitting activity in the visible light and the use of the composite in enhanced photocatalysis [41].

Simulations to investigate the electronic structure and photocatalytic performance of TiO_2 based-composites, hybrid DFT simulations are required. The results of these calculations indicate the alignments of energy bands, the mechanisms of charge transfer and photocatalysts in terms of light absorption, and inform the design of more efficient photocatalysts. Nanakkal and Alexander [42] focused on hybrid DFT by controlling the bandgap of a graphene/$BiVO_4$/TiO_2 nanocomposite [43]. These bandgaps coincided well, which they found across the heterojunction and facilitated efficient charge transfer. This alignment is essential to promote photocatalytic activity as it reduces recombination and makes it possible to produce reactive-species. The hybrid DFT study of TiO_2 composites by Yang *et al.* [44] concerned the electron-hole state distribution. They identified that addition of secondary materials reduced the bandgap of TiO_2 and spatially redistributed charge carriers to enhance separation capacity. The paper has focused on the manipulation of the electronic structure of the composite to achieve the maximum photocatalytic performance.

The synergy effect in TiO_2 composites is due to the joint action of its constituents. These effects consist of an increase in light absorption, enhancement in the separation of charge as well as an increase in surface reactivity [45]. The incorporation of graphene i.e. not only increases electronic properties but also provides adsorption sites of pollutants increasing reaction rates. The interplay between ceria and TiO_2 is seen to be the reason behind the success of Kumari *et al.* [46] in removing organic pollutants using ceria-tuned TiO_2 composites. Photocatalysis is further enhanced by coupling TiO_2 with noble metals (e.g. gold). Bhagya *et al.* [47] analyzed GNPs on TiO_2 composites and observed a steep increase in the absorption of visible light and charge separations efficiency. The bandgap of the composite was reduced to about 2.4 to 1 which gave larger spectrum of light. This is an improvement brought about by the plasmonic nature of gold that produces hot electrons and accelerates charge transfer.

Another synergy refers to Bi_2 Ti_2O_7/ $Bi_4Ti_3O_{12}$ nanocomposites examined by Du *et al.* [48]. The authors demonstrated that the bandgap of the composite and the morphology could be regulated by different temperatures of the calcination process and enhanced photocatalytic activity. The report emphasizes the optimization of the weaknesses in synthesis to attain the preferred synergies. Although this has become better, there are still challenges. Scaling up synthesis is one of the biggest challenges, because a good number of existing techniques are both time-consuming and expensive [49]. Composites also require improvement in terms of stability over long periods of illumination and extreme environmental conditions in order to be useful. Further experiments with computation tools may be combined with experimental research in the future to develop TiO_2 composites better. Machine-learning-based algorithms can hasten the discovery of new materials and can give an insight into the photocatalytic behavior. Also, commercial feasibility will be made through the development of inexpensive environmentally friendly synthesis pathways [10]. Summing up, TiO_2 composites are a promising path to eliminating limitations and enhancing the performance of pure TiO_2 and to improving the photocatalytic efficiency. These composites are a flexible system to use in environmental remediation and renewable energy technologies by exploiting single-phase interactions among a number of different materials. Design and optimization of these novel photocatalytic systems will still be directed by hybrid studies of DFT and TDDFT [50].

3. Separating Charges and Absorbing Light at Modified TiO_2 Systems

3.1 Separation efficiency Charge Carrier Dynamics

Better photo-catalytic activity of TiO_2-based materials requires better transfer of charge carriers and separate efficiency. When pure TiO_2 is used, the photons with energy equivalent to or higher than the bandgap generate electron and holes. It is anticipated that these carriers will promote a redox reaction of TiO_2 surface [51]. The problem with this is that the re combines with pure TiO_2, inefficiency of the overall photocatalytic rate goes down due to loss of energy to heat rather than reactions. New approaches are required to alter TiO_2 in a manner that recombination is suppressed and charge-carrier dynamics enhanced [52]. This part will explain the way charge carriers are formed, recombined, and apart in doped and composite systems of TiO_2 and how these influence the activity of photocatalysis. Photon absorption triggers carriers' creation in pure TiO_2.

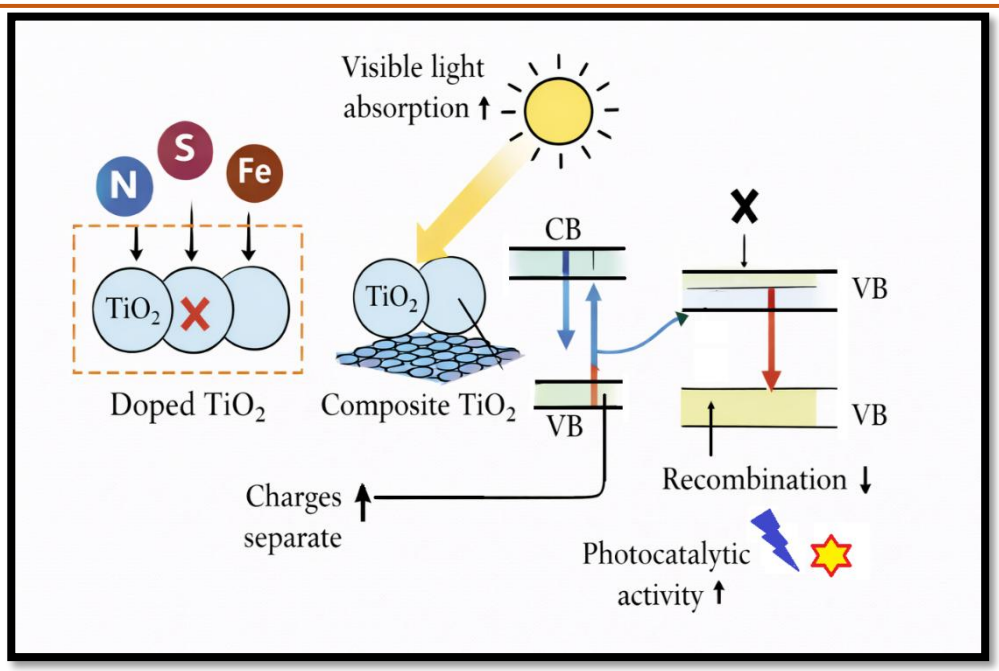

Figure 5. Separation of charges and light absorption in TiO_2 nanostructure.

A photon with energy sufficient (or more) to excite electrons generating a hole in the material (anatase TiO_2 has an energy bandgap of approximately 3.2 eV) causes an electron to be ripped off the valence band (VB) to the conduction band (CB). These electron-holes couples cause photocatalytic reactions [53]. The electrons in the CB can deprotonate oxygen molecules to superoxide radicals whereas the holes in the VB can oxidate water to hydroxyl radicals. Both pollutants are degradable in the presence of both reactive species.

This notwithstanding this limitation is due to the rapid recombination that usually takes place on the nanosecond timescale and decreases the spatial and temporal separation of carriers. Recombination may either be radiative (radiation) or non-radiative (heat). Best means to enhance the efficacy of photocatalytic processes are length of carrier proliferation and spatial segregation [54].

The chemically doped and composite are formed to alter the structure and electronic characteristics and inhibit recombination and promote separation, as shown in figure 5. Dopants form energy levels in the bandgap, which trap the electrons or holes and inhibits the instant recombination. TiO_2 composites heterojunctions may produce internal electric fields that accelerate electrons and holes in opposite directions thus enhancing spatial separation [55]. TiO_2 doping with foreign elements (e.g. cationic e.g. Fe, Al, W and anionic e.g. N, S, F) has been shown to be effective. Dopants cause mid-gap states or a change in VB and CB edges, changing the electronic structure of TiO_2 [56]. Indicatively, Samsudin and Abd Hamid [21] demonstrated that the bandgap is reduced and that co-doping with fluorine and nitrogen changes the dynamism of the charge. Electrons are trapped in the localized states and the two dopants to enhance photocatalytic efficiency by inhibiting their recombination with holes. These mid-gap states were confirmed by X-ray photoelectron spectroscopy and form the basis to separate the charges and enhance the absorption abilities of visible-light [50].

Likewise, Choi *et al.* [24] have explored the subject of tungsten doping and discovered that it lowers the recombination rate by behaving as an electron trap. W-doped TiO_2 exhibits a smaller bandgap and shows superior performance in selective catalytic reduction of nitrogen oxides. Measures of time-resolved photoluminescence showed that the carrier lifetimes were longer, proving of smaller recombination. In the study of doped TiO_2, Zhang and Xu [25] employed hybrid DFT computing. Their findings indicated that the spatial distribution of the charge density is altered by the dopants to form localized centers where the carriers dissociate and drift to reactive centers. These observations demonstrate the potential of lattice engineering to enhance the photocatalysis of TiO_2 with electronic Understanding in terms of its electronic properties. In addition to doping, the cut tough method of making TiO_2 with other materials is also a strong means of improving charge separation. TiO_2 forms heterojunctions with synergistic combinations (graphene, ZnO, or g -C_3N_4) to enable the spatial separation of electrons and holes [57].

Pasang *et al.* [26] have shown that the efficiency of charge-separation with TiO_2/graphene composite is better due to the high mobility of electrons in graphene. The hybrid DFT research study showed that at the interface, an electric field is created, which pushes the electrons of any crystal in the CB of TiO_2 to the graphene sheet, and leaves holes in the VB. This segregation decreases the recombination and enables

the carriers to engage their activity in photocatalytic reactions more fruitfully. Islam *et al.* [58] studied Al doping in the TiO_2/graphene composites, and it was possible to conclude that recombination was significantly reduced. Al dopants provide more energy levels which capture carriers and the graphene conductor allows transport of electrons. The experimental and theoretical findings indicate that the Al-doped composite is more active than pristine TiO_2 in the photocatalytic activity.

Ren *et al.* [59] fabricated Ti^{3+}- doped TiO_2 composites, which showed better performance. Ti^{3+} ions form oxygen vacuoles which trap electrons and the composite structure facilitates carrier movement. The paper has focused on $NaBH_4$ as reducing agent which can regulate doping content, as it has a direct effect on charge separation processes, and photocatalytic performance. TDDFT has emerged as an important computational technique in the study of the dynamics of charge transfer and charge separation in the reduced TiO_2. TDDFT simulations give detailed information on electronic transitions and charge-transfer reactions defining photocatalytic reaction. Ullah *et al.* [28] studied WO_3 doped TiO_2 catalysts with the help of TDDFT. It was found, based on the simulations, that W dopants provide a continuum of mid-gap states which facilitates the movement of electrons to the CB and holes remain localized in the VB. This segregation lowers crossbreeding and increases efficacy. The report also demonstrated the concentration of the dopant changing the charge transfer, where the highest activity was found at the optimal concentration. Nair *et al.* [31] researched TiO_2/ZnO included composites by TDDFT. They found that the heterojunction provides a staggered band gap, with electrons flowing in the CB of ZnO to the CB of TiO_2, and holes flowing the other way around. This separation of charge is based on the disparity of electron affinities and ionization potential of the two materials, which is anticipated in TDDFT. The results indicate the challenges of aligning the band in creating effective photocatalyst.

In their simulation, Munir *et al.* [32] used TDDFT to study the influence of carrier concentration on separation in doped TiO_2. They discovered that past a certain dopant concentration there are recombination centers formed to reduce efficiency. The simulations provide a theoretical model of doping level plus carrier controlling, which focuses on the perfect control on incorporating dopants. In a nutshell, the design of TiO_2 systems by altering them via doping and composite formation is of paramount importance in improving kinetics and separation of charge-carriers. Dopants add onto the localized levels of energy which inhibit recombination and composites form heterojunctions which enhance the spatial segregation between the electrons and holes. TDDFT innovations can be used to gain a better insight into charge-transfer processes and selectivity, and this understanding can be used to design highly-performing photocatalysts. Through optimization of these adjustments, TiO_2 based materials have the potential of being optimized to acquire greater photocatalytic properties and further in environmental cleanup and energy transformative technologies [57].

3.2 Absorption Spectrums of Light through TDDFT

The capacity to utilize the visible light is vital to the photocatalytic capacity of titanium dioxide (TiO_2)-based platforms. The chemical stability of pure TiO_2 is also non-toxic, and the wide bandgap (i.e. 3.2 eV for anatase) absorbs only ultraviolet (UV) light, a distant portion (i.e. 5 percent) of sunlight [60]. Investigators have thus made attempts to change TiO_2 in a way that it can absorb visible light. TDDFT is a robust computational method that is able to predict the absorption spectroscopy and also elucidates the electronic transitions in doped and composite TiO_2 [22]. TDDFT simulations provide a conceptual framework of examining the effect of doping or composite formation on the electronic structure and optical properties of TiO_2. TDDFT can determine the exact transition that is active in the visible-light by modeling the dynamics of the excited-states and the calculations of the spectra. In this section, an account of TDDFT principles, prominent doped TiO_2 practice and composite systems, and the ability of these to exhibit enhanced light absorption are demonstrated, and computational forecasting relative to experimental outcomes is discussed, which justifies the practice [61]. Time-Dependent Denis Functional Theory, Time Dependent DFT which presents the excited states as extensions of ground-state DFT. TDDFT computes absorption spectroscopic data using time dependent Kohn Sham equations which incorporate electronic excitation. The simulations indicate the levels of energy, the strengths of oscillators and the probability of transition, and they can be used to predict ways in which alterations of the electronic structure of TiO_2 affect its optical characteristics [62].

Another essential feature of TDDFT is its ability to solve individual electronic transitions, such as those that are caused by dopants or heterojunctions. To draw from a few examples, the dopants providing mid-gap states can cause new absorption bands in the visible range whereas in heterojunctions in composites, charge-transfer transitions can be enhanced. The possibility to establish such transitions provides a clear way forward in the rational engineering of TiO_2 materials that have the most effective light-harvesting behavior. One of the widely considered ways to reduce the bandgap of TiO_2 and broaden its absorption to the visible range is doping. Both the anionic and the cationic dopants may bring about localized states or an

approximate shift in band edges. The simulations based on the TDDFT are critical to the explanation of the impact of particular dopants on the electronic structure and absorption of TiO_2.

As an example, Samsudin and Abd Hamid [21] reported that co-doping TiO_2 with nitrogen (N) and fluorine (F) led to a decline in the bandgap to approximately 0.952 eV. TDDFT indicated that the reaction between N and F formed mid-gap electronic states which increased the absorption of VL. X-ray photoelectron spectroscopy (XPS) verified the changes in electronic structures which were proposed by TDDFT. This example illustrates the effectiveness of using dopants in combination compared to using individual elements of doping. Ullah *et al.* [28] examined the tungsten (W) doping in TiO_2. TDDFT has shown that W brought in donor states close to the conduction band due to which the bandgap has been narrowed, which allows the absorption to expand to the visible frequency range. Computational predictions were validated by experiments that demonstrated that W-doped TiO_2 had enhanced visible-light photocatalytic activity to degrade Congo red. This paper highlights the usefulness of TDDFT in the design of doped TiO_2 with specific optical characteristics. The other strategy that proves to be effective in enhancing the light absorption and photocatalytic activity of TiO_2 is composite formation. Heterojunctions have been formed by combining TiO_2 with other materials like graphene, ZnO, or g-C_3N_4, which allow transfer of charge and has increased the spectrum of absorption. The TDDFT simulations are useful in the study of the electronic interactions at the heterojunction interface and in the determination of the optical behavior that results.

Nair *et al.* [31] have studied TiO_2 mixed and non-metallic doped and co-doped materials. TDDFT showed that the creation of a continuum of mid-gaps by the formation of the heterojunctions greatly increased the ability to absorb visible light. Their investigation revealed a synergistic effect on the enhancement of the optical properties of TiO_2 due to the presence of doping and composite formation. Mollavali *et al.* [63] investigated the co-doping of TiO_2 composites with various cationic and anionic elements. TDDFT indicated that co-doping had a large range of electronic states in the bandgap resulting in a redshift to the absorption spectrum. The enhanced photocatalytic performance of the co-doped composites was experimentally established, particularly in the production of hydrogen and degradation of a pollutant. One of the problems of computational material science is to bridge the gap in theory and experiment. In the case of TiO_2 systems TDDFT has always given the correct prediction on the absorption spectrum which has been consistent with laboratory results. Zhang [25] reported that changes in the lattice and the area of the surface can be used to tune the bandgap and increase the effectiveness of photocatalysis. Their TDDFT calculations performed enhanced visible -light absorption in TiO_2 with a lattice architecture structure. The calculations of experimental absorption and activity values were similar to the computational results, which depicts the reliability of TDDFT.

Ren *et al.* [59] targeted Ti^{3+} doped TiO_2, in which Ti^{3+} gives additional electronic levels into the bandgap. TDDFT estimated an enormous increase in the absorption at visible light, which was checked by UV-Vis spectroscopy. Understandings of the manner in which the Ti_{3+} dopants modify the electronic structure were used to design TiO_2 materials with better optical characteristics. TDDFT has further developed knowledge of the altered TiO_2 system with the detailed knowledge of the electronic transition and energy state which contributes to the visible-light activity. As can be seen in the above explanations, doping and composite formation have the potential to decrease the bandgap and enhance light absorption in TiO_2. There are, however, certain problems. Some more efforts would be needed in scaling computational predictions to real world systems as well as combining TDDFT with experimental techniques. The next generation of research needs to construct more advanced models such as the inclusion of dynamic effects such as phonon effects and surface defects that can provide even more precise predictions of optical and photocatalytic properties. To conclude, TDDFT is an effective method in predicting and optimization of light absorption in doped and composite TiO_2 system. With the development of the computational means, they will be the simultaneous subject of interest to carry out the experimental studies, developing photocatalysis and resolving the global energy and environmental issues.

4. Photocatalytic Efficiency and Pathways in Degradation of pollutants

4.1 Reactive Pathways of Degradation of Pollutants

Degradation of pollution in photocatalytic systems is a complicated process with numerous chemical reactions. These reactions dissolve toxic pollutants into minor harmless or neutral substances. TiO_2 has long been considered to be a good photocatalyst due to its chemical stability, being non-toxic and very active in UV light [64]. Nevertheless, it is not very effective in visible light due to the large bandgap (approximately 3.2 eV of anatase TiO_2). The researchers have thus been keen on changing TiO_2 through doping or creating composites. These changes increase its chemical catalytic efficiency particularly in pollutant degradation. This section describes typical degradation mechanisms, the impact of dopants and composites on them, and computational and experimental studies examples that have combined the

changes on TiO_2 to the pollutant-degradation efficiency [19].

The purification of pollutants using TiO_2-based photocatalysts principally depends on the reactive oxygen species (ROS) generation. These are; hydroxyl radicals (•OH), superoxide anions (O_2) and singlet oxygen (O_2). ROS are incredibly reactive and have the ability of breaking complex organic pollutants into simpler and less toxic compounds including CO_2 and H_2O [65]. The photocatalytic reaction begins with the light activating the electrons in the valence band (VB) to the conduction band (CB) of TiO_2, and vacating the VB. These electron-holes pairs in turn promote redox reactions on the catalyst surface. Using the case of holes, they may oxidize water or hydroxide ions and produce •OH radical or reduce molecular oxygen and produce O^{2-}. The pollutants are decomposed primarily by ROS. As organic molecules, hydroxyl radicals particularly are effective in breaking chemical bonds thereby resulting in mineralization [66]. The total efficiency is conditional on a number of factors: charge-carrier separation and movement, the available active sites on the surface and the nature of the pollutant. The addition of dopants (anionic and cationic) and the formation of TiO_2-based composites have a significant impact on the degradation mechanisms. These alterations change the electronic structure, light absorption and surface chemistry of TiO_2. Dopants have the ability to form mid-gap states, smooth out bandgap, and enhance the process of absorbing visible light, and thereby expand the activity of TiO_2 in the visible spectrum. Heterojunctions may stimulate the processes of charge transfer and decrease recombination through the utilization of composites.

4.2 Solvents Anionic and Cationic Dopants

Nitrogen (N) and fluorine (F), which are anionic dopants, add localized states above the TiO_2 bandgap. It was demonstrated by Samsudin and Hamid [21] that N and F co-doping yields a synergetic effect and decreases the bandgap to approximately 0.95 e V. This enhancement increases absorption in visible light and generation of ROS during the case of sun irradiation, which enhances the rate of pollutant degradation. Transition metals such as tungsten (W), tin (Sn) and iron (Fe) are cationic dopants. They insert states to the conduction band or its boundary. According to Bhagya *et al.* [47], Sn_2TiO_2 nanocomposites showed increased photocatalytic behavior, with a rate of 216.5 0 0mol hydrogen evolution. This lead is attributed to the fact that Sn can be used to tune the phase and crystallite size of TiO_2 enhancing the production of ROS to be used in the degradation of pollutants. Islam *et al.* [29] discovered that the Al doping of TiO_2 finite films enhances photocatalyst structure and morphology hence enhancing the photocatalytic activity.

4.3 Composite Materials

TiO_2-based composites are materials that have numerous combinations of materials to enhance photocatalytic activity. As an exemplar, when TiO_2 is attached to graphene, ZnO, or g-C_3N_4 heterojunctions are formed that tend to separate charges and collect light more efficiently. Ullah *et al.* [28] examined W-doped TiO_2 composites in terms of breaking down the Congo red dye. They discovered that even the 6 mol.% tungsten dosage is much more effective with regards to shows of activity when visible light is utilized. The article demonstrates that dopants and compounds are able to contribute to increasing the breakdown of pollutants by maximizing the absorption of light and carrier transfers. The efficiency of TiO_2 modification in the process of pollutants degradation has been extensively studied by using both computational and experimental approaches. Hybrid density functional theory (DFT) and time density DFT (TDDFT) provide information on electronic structure, light absorption, and reaction pathways of modified TiO_2. These pre-emptive opinions can be verified experimentally to form a formidable system of knowledge and control of the TiO_2 photocatalysts.

As an example, Zhang and Xu [25] applied hybrid DFT to determine the influence of lattice strain and surface area on the bandgap and efficiency of TiO_2. Their findings highlight the importance of electronic structure and surface property modification of TiO_2 to enhance the degradation of the pollutants. On the same note, Mollavali *et al.* [63] tested the co-doping of TiO_2 with various cationic and anionic elements. They discovered that this type of co-doping yields synergistic action increasing the photocatalytic efficiency. These results are backed up by experimental studies. Nair *et al.* [31] demonstrated that co-doping with metal and non-metal reduces the bandgap of TiO_2 such that it becomes active at visible light, and the rate of pollutants break-down accelerates. The article by Yang *et al.* [44] focused on surface chemistry in TiO_2 photocatalysis. They established that metal doping forms in the inside of the bandgap, thereby enhancing the charge carrier dynamics and production of reactive oxygen species (ROS). Another evident example was given by Ren *et al.* [59] who examined Ti^{3+} doped TiO_2. They demonstrate in their work that with the help of the control of the dopant quantity and the environment of the reactions, the performance could be optimized. Addition of Ti^{3+} to the bandgap increases the absorption in the visible-light and the degradation speed.

The rate constants of degradation, quantum efficiency, and percentages of pollutants removed are some of the measurements commonly used to compare modified TiO_2 photocatalysts. The article by Wang *et al.* [67] explored Sn anatase-rutile composites and documented significant enhancement in the

degradation of organic pollution. The findings by them highlight the role of phase composition and nano-dopant caused narrowing of the bandgap. In another study, Mollavali *et al.* [63] established that co-doping of TiO_2 with several elements gives a better performance with regard to the breakdown of industrial dyes and pharmaceutical pollutants. The authors explain such an improvement by the presence of dopant synergy, which facilitates the light absorption, charge-carrier processes, and the generation of ROS. Many difficulties are still there despite the envisioned improvements. It is not easy to scale doped and composite TiO_2 systems to real world application and stability when dealing with long-term operation is uncertain. Besides, the sophisticated interaction between a dopants, composites, and surface chemistry needs to be studied in greater detail so that to optimize photocatalytic performance. The development of new computational tools should be combined with experimental research in the future to gain a better insight into the mechanisms of degradation. The combination of the best dopants and operation conditions could be predicted by machine-learning algorithms. Moreover, new paths of efficient and green pollutant degradation may be made available by designing new TiO_2 -based composites with specific properties. To sum up, it is concluded that doping and composite formation is an effective approach to form TiO_2 into improving its ability to photocatalytically decompose pollutants. Such a comparison can help engineers develop superior photocatalysts that address the challenges impacting the environment and serve as a sustainable technology.

4.4 Surface Chemistry Role in Photocatalysis

To operate as photocatalysts, TiO_2 materials require surface chemistry. A scientific breakthrough enables scientists to increase the surface properties to enhance the reaction of reactants between the catalyst and this is an advance in improving the breakdown of pollutants and other photoreactions [68]. It is this changes in the surface that can impact photocatalysis, the role of adsorption sites and charge, and what hybrid DFT simulations can say about reaction energies on modified TiO_2 surfaces that is examined in this section. Increasing TiO_2 activity is used by surface modifications; such as the addition of co-catalysts or functional groups. These alterations influence surface area, charge distribution, and density of active site, which respectively impact on reaction efficiency. According to Samsudin and Hamid [21], the addition of nitrogen and fluorine as co-dopants in TiO_2 reduced the bandgap by approximately 0.95 eV, enhancing its absorption in the visible light and decreasing photocatalytic activity. The advantage was associated with the emergence of new surface states which favored charge transfer and decomposing pollutants. According to Zhang and Xu [25], the bandgap can be tuned by larger surface area and lattice alterations and enhance photocatalysis. The catalyst enhances the escalation of the pollutants by increasing surface area and active sites, which increases the rate of degradation. According to these results, surface modifications that are made in the optimum way to ensure that both electronic and structural properties can be used in the most efficient way to utilize light and catalysis should be developed. Bhagya *et al.* [47] have investigated the doping of tin (Sn) in TiO_2 nanocomposites. The development of 5% Sn addition did not only increase the performance but also it changed the surface chemistry. Sn generated new active sites, assisted the transfer of electrons, as well as minimized recombination. This change of the surface lead to the increased capture of pollutants, which increased photocatalytic activity even more. These results support the fact that surface transformations contribute to the overall performance of TiO_2.

The reactions in the photocatalysis field are dependent on the surface density and the functionality of the adsorption sites of the catalyst. It is these sites that are the primary points of contact between the catalyst and reactant molecules that allow transfer of electrons or radicals required to degrade. Ullah *et al.* [28] have provided the evidence that the tungsten (W) doping has led to the increase of adsorption sites and the enhancement of charge characteristics in the surface that enhanced the extent of light absorption and the powers to degrade the Congo red. The enhancement was brought about by an enhanced contact of the pollutants and the modified TiO_2 surface. The surface charge also determines the manner in which pollutants react and degrade. Negatively charged pollutants adsorb well on positively charged surfaces and vice versa. Mollavali *et al.* [63] examined the co-doping of using various cations and anions (or having a balanced distribution) to obtain a balanced charge distribution. This increased its adsorption capacity and facilitated segregation of charges to minimize recombination. Their article demonstrates that photocatalytic reactions can be enhanced using a tuned charge environment.

Hybrid DFT simulations can be relied on to inform the researcher about the dynamics of surface chemistry changes on the activity of TiO_2. In Nair *et al.* [69], the hybrid DFT was employed to investigate the metal and non-metal doping. According to the simulations, the introduction of doping in mid-gap states and also shifting electronic states towards the edge of the band altered light absorption and charge-transfer characteristics. Such changes also reduced the activation energy of the degradation of pollutants. The analysis with hybrid DFT proved to be useful in the study of TiO_2 doped with metal as confirmed by Yang *et al.* [44]. They discovered that metal dopants form

localized conditions within the bandgap and enhance the source of interaction between TiO_2 surface and reactants. This alters reaction energetics to allow enhanced charge transfer and radical generation which enhances performance. These findings demonstrate the way in which hybrid DFT could be used to inform surface-modification design.

Ren *et al.* [59] performed the study of TiO_2 with hybrid DFT, wherein Ti^{3+} is doped. They found that Ti^{3+} produces a steady series of surface species which serve as active sites in pollutant degradation. These states favor the appearance of hydroxyl radicals and other reactive species necessary to do photocatalysis. The significance of manipulating surface states to enhance the reactivity and efficiency of TiO_2 is insisted on in the work. Wang *et al.* [67] studied the surface alterations of Sn-doped anatase-rutile TiO_2. They discovered that the inclusion of Sn enjoyed better light absorption as well as promoting surface chemistry through the inclusion of active sites and reconstitution of charge distribution. Such modifications greatly enhanced the degree to which organic pollutants were degraded, demonstrating the possibility of surface engineering to make TiO_2 more useful. A combination of experimental data and the hybrid simulated DFT provides a good foundation to grasp the surface chemistry of photocatalysis. Through the ability to adjust surface characteristics, researchers are able to develop better TiO_2 systems to absorb more light, separate charge more efficiently, and degrade pollutants more prolifically. Future studies ought to combine the best computation methods with laboratory methods to further improve the surface modifications and to utilize the full potential of TiO_2 as a photocatalyst.

5. Outlook and Shortcomings

The use of doping and making composite is being explored by researchers to enhance the photocatalytic properties of titanium dioxide (TiO_2) [70]. These plans can address the inherent limitations of TiO_2; its broad bandgap (3.2 eV and above) to visible light absorption and its high recombination rates between electrons and holes. Backed by hybrid density functional theory (DFT) and time dependent density functional theory (TDDFT) simulations [71], the contemporary literature elucidates the impact of dopants and composite materials on electronic frameworks, expansion of light absorption out to the visible domain, and charge partition. Doping (anionic, i.e. nitrogen or sulfur), or cationic (i.e. iron and tungsten) doping causes a filling of the mid-gap states or an alteration of the band edges so that the bandgap becomes narrower. In fact, Choi *et al.* [24] demonstrated that doping with tungsten narrowed the bandgap, and made TiO_2 more active in the visible light. In addition, Zhang and Xu [25] emphasized that lattices alteration with the help of dopants serves as a major factor in bandgap tuning, as they alter the electronic environment of TiO_2 and its surface area, which enhances the photocatalyst on TiO_2. The composite formation makes use of the synergistic nature of TiO_2 with other materials like graphene, zinc oxide (ZnO), and graphitic carbon nitride (g-C_3N_4). These heterojunctions provide electrons and holes with separate paths which reduce the recombination rate. According to Pasang *et al.* [26], defect engineering in such composites additional tunes the bandgap and increases the photocatalytic activity. A difference study by Yun *et al.* [72] on the impact of substrates and surface modification on optical bandgap indicated that composite systems could be adapted to the specific use.

These advances still pose a problem. Computational predictions are challenging to scale to realistic applications and theoretically, the models are challenging to validate. To close these gaps, researchers such as Fidalgo *et al.* [73] argue that a more integrated methodology, which tries to combine computational models with high-end experimental methods, is needed. Although it is possible that TiO_2 modifications have full potential, the field suffers a few shortcomings that can inhibit the practical application between research and commercial development. These drawbacks can be categorized as computational, experimental and material constraints. Hybrid DFT and TDDFT simulations are extremely useful in making predictions of the impact of doping and composites on TiO_2. They are however computationally intensive and most of the time they tend to consume large amounts of resources to model complex systems in a good and accurate fashion. Islam *et al.* [29] remarked that in spite of the fact that hybrid DFT provides further accurate information about the band structure, it is not yet used in large-scale or real-time dynamics. Also, the inaccuracies of DFT and TDDFT are likely to lead to a discrepancy between prediction and observation particularly with high disordered or defect rich material.

The other constraint is that computational models are not scalable. The vast majority of simulations consider the idealized case of systems and perfect crystalline structures, which are not necessarily applicable to real materials that contain defects, impurities and surface irregularities. Munir *et al.* [32] pointed out that these defects play a significant role in the photocatalytic activity of TiO_2 and are usually not considered during theoretical research. To bridge this gap, stronger methods of computation should be used, which take into consideration the heterogeneity of materials. Computational predictions are still subject to experimental validation which is a serious bottleneck. Though hybrid DFT and TDDFT provide a theoretical basis, the translation of these results into more useful materials often requires very much trial and error work.

Qi *et al.* (2021) concluded that heterostructure photocatalysts with theoretically optimized bandgaps had practical limits in their synthesis and stability that impeded their use.

One important concern is the ability to reproduce the experimental findings. The differences in synthesis procedures, environment, and material properties may cause different results thus making it hard to validate. As mentioned by Khani *et al.* [74], the absence of standard procedures regarding doping and composite formation deteriorates this problem, and it is difficult to compare the results in the literature. It is also difficult to describe modified TiO_2 systems. Examples of the methods that can offer practical structural and optical information include the X-ray diffraction (XRD), scanning electron microscopy (SEM), and UV-Vis spectroscopy, which might lack the depth of charge dynamics and surface interactions. Sophisticated techniques such as ultrafast spectroscopy and in-situ monitoring are required to mitigate this gap but they are expensive and are not readily available to most users. The intrinsic character of TiO_2 and its altered forms also become an obstacle to their practical use. As an example, although doping may have the advantage of reducing the bandgap it frequently creates levels that are defects, which are recombination centers to the detriment of enhanced light capture. Sakar *et al.* [75] remarked that the introduction of dopants should be strictly regulated in order to strike a balance between the trade-off between the reduction of the bandgap and the recombination rates.

Likewise, although the concept of composite formation is viable, it has challenges in terms of compatibility and stability of the material. The surface between TiO_2 and other substances within a compound system is a very important factor in charge transfer capability. Nevertheless, it can be difficult to stabilize a working and efficient interface, as lattice structures, thermal expansion numbers and chemical reactivity often vary. As Yun *et al.* [72] emphasized, even a small interface mismatch may result in a high rate of recombination and low photocatalytic activity. The scalability of synthesis methods is another limitation associated with materials. Some of the techniques such as sol gel processing, hydrothermal synthesis, and chemical vapor deposition are effective at the laboratory level but might not be applicable to scale production since they are very expensive, complex and environmentally disadvantageous. This scaling problem is especially applicable to those applications that are based on high amounts of photocatalysts, like water purification and air filtration. To resolve these drawbacks and release the maximization of modified TiO_2 systems, any future study has to take a multidisciplinary perspective where advanced computational schemes, new manufacturing methodologies and strict experimental checking are implemented. The following are some of the promising directions.

Among the most urgent issues, it is the creation of the integrated frameworks incorporating the computational modeling and experimental research. The style has the potential to close the divide between theory and practice giving a better idea of the material properties and the photocatalytic behaviour of materials. Indicatively, Fidalgo *et al.* [73] proposed applying machine-learning algorithms to the analysis of large datasets produced by hybrid DFT simulations, which allows predicting high-quality doping and composite. Also, replication of real-life conditions in computational models may make them more relevant and true to life. As an example, Zhang and Xu [25] suggested the use of factors such as temperature, pressure, and surface roughness in DFT simulation to be more realistic of experimental environments. In a similar manner, Munir *et al.* [32] recommended multi-scale modelling methods that comprised both atomistic and continuum-level analysis, where they can give a more holistic description of a material behaviour.

The manufacturing of materials of the innovations is a key to making the most of doping and composite forming limitations. The application of the green chemistry methods to create cost-effective and environmentally friendly methods to synthesize is one of such directions. Indicatively, Khani *et al.* [74] examined the application of bio-inspired methods in doping TiO_2, and the researchers made attempts to utilize the natural processes to obtain the control of the location and concentration of dopant with high precision. The other area of focus is on the growth of self-assembling composites whereby the constituents architect themselves to the required structure without undergoing the complicated processing steps. Qi *et al.* [76] also indicated that the self-assembly methods might be especially efficient to produce heterojunctions with a defined interface, which would spectrally separate charges and increase the photocatalytic conversion. More complex characterization methods are needed to further reveal the characteristics of the controlled TiO_2 systems and be able to prove the computational anticipations. An example is in-situ methods that have the capability to monitor photocatalytic reactions in real-time, which can inform charge dynamics, surface reactions and pathways of reactions. Sakar *et al.* [75] emphasized the possibilities of time-, spectroscopy, to measure the ultrafast electron and hole dynamics and have a better insight into the recombination mechanisms.

6. Conclusion

The structural and morphological characteristics of doped and composite TiO_2 systems on the nanoscale can be observed with the assistance of the development of the high-resolution imaging

techniques, including atomic force microscopy (AFM) and transmission electron microscopy (TEM). These findings can be used to design more efficient photocatalysts by establishing the most important criteria to be used in designing the photocatalysts. Lastly, use of new materials and configurations not restricted to conventional doping and composite approaches should involve future studies. Indicatively, this has been demonstrated by the recent promise of the application of plasmonic nanoparticles to improve light absorption due to localized surface plasmon resonance (LSPR). Photocatalytic activity of TiO_2 systems could be intensified significantly due to the introduction of gold or silver nanoparticles in the system to expand light absorption into a near-infrared range.

The other emerging trend is the innovation of multi component systems, which integrate the capabilities of different materials. As an example hybrid systems, such as TiO_2 with metal -organic frameworks (MOFs), or covalent organic frameworks (COFs), may have distinct benefits, such as, enhanced light harvesting, charge separation, and pollute adsorption. General, the current strategy of doping and composite creation of TiO_2 to increase its photocatalytic activity is worthwhile. These techniques have shown a great deal of improvement in light absorption, charge separation, and reaction dynamics with the help of hybrid DFT and TDDFT simulations. But computational scalability issues, experimental validation and material properties will have to be surmounted to allow full exploitation of these systems. Future studies ought to concentrate on combining computational and experimental methods, creation of superior synthesis and characterization methodologies and on new materials and structures. The development of the multidisciplinary approach can be used to address the existing constraints and open the door to the next generation of TiO_2 based photocatalysts, and it can find its application in areas such as environmental cleanup and renewable energy production. The process leading to this end, though not without many obstacles, has tremendous potential of addressing some of the most burning global problems of today.

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