



Review

Photo-to-chemical energy transformation: Pioneering photocatalysts, surface and interface engineering

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ABSTRACT

Photocatalysis entails materials that have specific features for widespread practical applications, including, powerful light absorption, rapid charge transport, an adequate band assembly, and high quantum efficiency in a substantial and definite surface area. The concept of "photochemical potential" is presented on the evidence of using photons as reactants. Now, it can be expressed in the terms "photocatalytic" and "photosynthesis" by referring to all light-induced catalytic activities. These events are mutually spontaneous reactions observed in the allied physical domes. Elementary research practices used to improve the photocatalytic capability of the photocatalysts include innumerable cutting-edge processes such as surface modification, doping with metal or non-metal components, and band gap modification. These techniques can reduce promoted oxidation, photo-induced charge carrier ability, and increase light absorption, but during investigations, the photocatalytic quantum efficiencies and interfacial charge mobilities of the photocatalysts continue to be low and inadequate. It is crucial to create effective photocatalysts that can perform rapid charge separation, high quantum efficiency, and robust light absorption. This succinct analysis examines the timeline of substantial photocatalysis discoveries and offers an overview of current knowledge on the discussed phenomenon. A mathematical expression for photocatalytic degradation was developed and substantiated as a part of this review covering the current needs. It is a forward-looking approach applied to outline the reaction routine and its progression route. This work offers a straight-forward outlook for forecasting how well a photocatalytic system will perform in terms of deterioration. A minimum reliance on experimental data and the absence of adjustment factors lead toward a planned approach. The authors provided mathematical equations as a new constraint to analyze mathematical modeling, probability, evaluation of the photocatalytic degradation for revisiting the definition of photocatalysis, analyzing energy bands and energy levels, and finally the Monte Carlo simulation and transpired simulation described. The analogy analysis of electro catalytic water splitting was also included. The probability and apprehensive aspects of a photon have been immersed by photocatalytic suspension and how it will produce an oxidizing agent is further derived through mathematical derivations. Finally, the probability depends only on the photocatalyst performance particularized mathematically.

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1. Introduction

Solar energy, which is the primary kind of energy obtained from space, can significantly outpace the world's annual energy needs. Solar energy is the highest-quality renewable resource that can be harvested on the planet Earth due to the Sun's expected long lifetime. Despite this, there are major difficulties in harvesting, storing, and using this energy source because it is intermittent and daytime-only. The photovoltaic effect, which was first discovered in 1839 and is attributed to Edmond Becquerel, may be the method of solar photon harvesting that has been the subject of the most research [1]. To achieve the sustainable development objectives put out by the United Nations, photocatalysis is an encouraging technique for effectively converting and storing solar energy. The technologies that are currently available can be used to resolve these complications. As an illustration, solar energy can be directly captured, transformed, and stored as heat, which can either be used to heat a home or converted it into electricity later. The definition of photocatalysis, despite nearly a century of research on the subject, is still up for debate. Whereby photosynthesis and photocatalytic differ significantly. In this succinct assessment, the history of substantial photocatalysis discoveries is scoured, and the current state of knowledge concerning photocatalysis is refined [2]. The definition of photocatalysis is revised and given using the electrocatalysis as an analogy. Thus, photocatalysts are thought to be a promising and environmentally acceptable technology for converting solar energy into thermal or chemical energy through interactions with light matter.

To refer the photons as reactants, the phrase "photochemical potential" is proposed. In light of the fact that both the debatable "photocatalytic" and "photosynthetic" procedures are extemporaneous responses transpired during relevant somatic domains, it may be concluded that photocatalysis is the general term for all light-induced catalytic activities. Heterogeneous photocatalysis using semiconductors has drawn a lot of interest as a green and ecological expertise recently due to its potential to resolve energy and environmental issues [3]. The green technology that has been widely used to address energy and ecological problems is semiconductor-mediated photocatalysis. By using various surface changes, photocatalytic effectiveness is increased. As a result, the mechanisms of visible-light-active photocatalysts' photocatalysis have been described. These mechanisms involve changes in the semiconductor's band-gap structure brought about by adsorption modifiers (surface modification) or band-gap narrowing (doping), respectively (Fig. 1). Visible light response is shown because of heterojunction between the two semiconductors [4]. Due to the interesting

advantages in increasing light-harvesting in surface reactions occurred during charge transfer dynamics in a photocatalytic assembly, the single-atom photocatalysts have proven its convincing potential probably in establishing analysis of greatest energetic route transpired during photocatalysis. Thus, a thorough discussion of novel photocatalysts, including metal-organics, metal oxides, graphitic carbon nitrides, metal sulphides, and graphene describes significant surface/interface phenomena involved in photocatalysis, such as the Z-scheme system and surface heterojunctions have been illustrated [5].

Examines the operation of co-catalysts and the process of adsorption on photocatalyst surfaces, and it is edited by leading interface scientists from all over the world. Succeeding a basic introduction to single-atom photocatalysts, the assistances and uses of these catalysts in photocatalysis are delivered. For a variety of uses, including the production of solar fuel and the degradation of environmental contaminants, heterogeneous photocatalysis has been thoroughly studied as a viable and promising approach. For use in practical applications, it is currently difficult to create highly selective, active, and long-lasting photocatalysts. After giving a brief overview on the history of photocatalysis here, authors provide a thorough analysis of photocatalysis's thermodynamics and dynamics, which can greatly aid readers in understanding the underlying concepts behind photocatalytic processes [15]. The fundamentals of the surface/interface science of photocatalysis are then succinctly reviewed by including, interfacial charge separation, surface redox reactions, and covering topics such as adsorption. The modification tactics, and methodologies for characterizing, designing philosophies and evaluating semiconductor photocatalysts are compiled (Fig. 2).

Next division on water splitting, synthetic chemistry claims, and environmental photocatalysis, more this reviews concentrate on creating and designing photocatalysts, environmental issues, and solar energy transformation and the photocatalytic transformation of CO₂. Metal/semiconductor and nanostructures as photocatalysts have been rationally designed and synthesized owing to advancements in theoretical and investigational revisions on plasmon-mediated photocatalysis [17]. Numerous hybrid nanostructures have reported by combining inorganic and organic surface modifications, heterojunctions, and dopants. The synthesis of SPR-based materials using a recently described, simple process is highlighted along with significant advancements in plasmon intervened photocatalytic routes, including Schottky junctions, nonstop electron transfer, improved native electric field, plasmon resounding energy transference, scattering and heating paraphernalia (Fig. 3) [18].

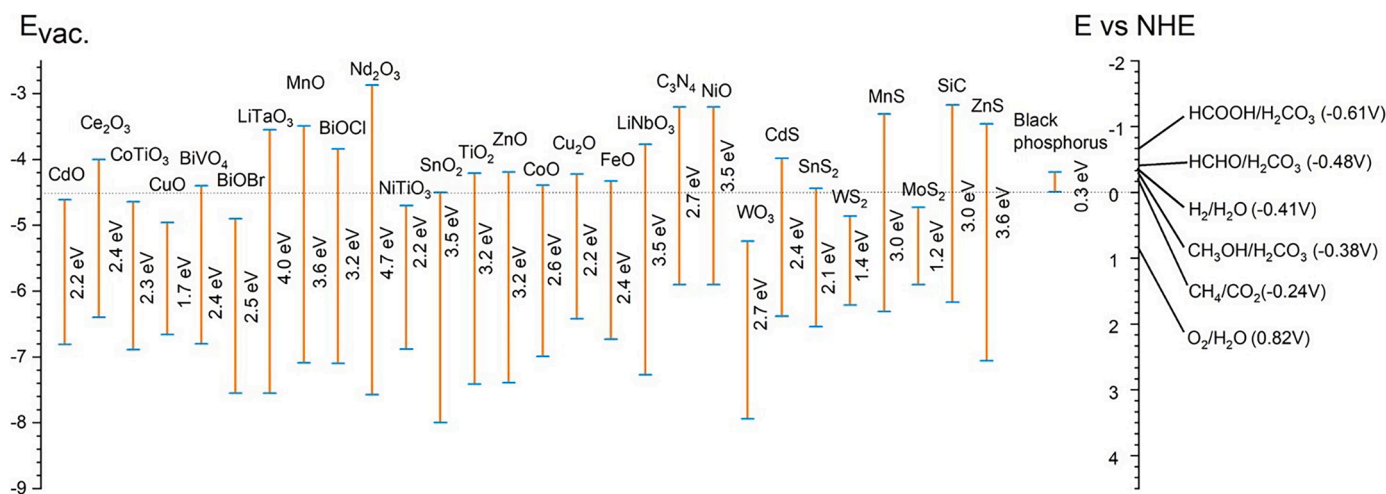


Fig. 1. Band edge locations at pH = 7 of several photocatalysts in relation to different redox potentials. A diagram showing the band edge positions according to Refs. [6–13]. Reprinted (adapted) with permission from Ref. [14]. Copyright (2016) Aleksandra B. Djurišić et al. APL Materials, AIP. Open Access under the terms of the Creative Commons CC-BY License.

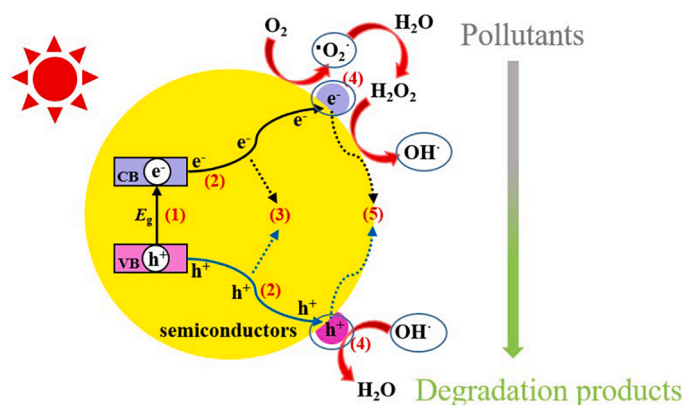


Fig. 2. A schematic illustration photocatalytic processes during a heterogeneous photocatalysis. Reprinted (adapted) with permission from Ref. [16]. Copyright (2021) Zizhen Li et al. Nanomaterials (Basel), MDPI. Open Access under the terms of the Creative Commons CC-BY License.

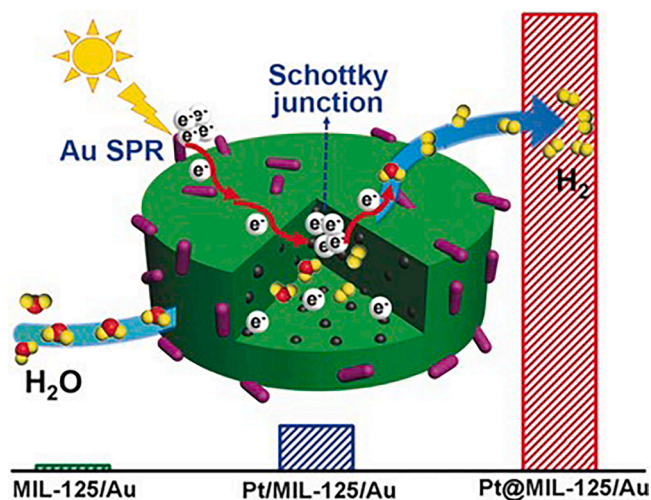


Fig. 3. Schematic illustration of Schottky junctions into metal-organic framework composites. Reprinted (adapted) with permission from Ref. [17]. Copyright (2017) Hai-Long Jianget al. Angewandte Chemie, John Wiley & Sons, Inc. Open Access under the terms of the Creative Commons CC-BY License.

Numerous understanding of single-atom photocatalysts have lately been accrued, but cutting-edge depiction approaches and important theoretical research that are deepening knowledge related to refer stimulating materials, enabling current views to predict the operational capacity of these tools in photocatalytic assertions. For this review, authors chose articles from the Web of Science database that span almost fifteen years, with most our sources covering the last eight years [19]. The current review compiles the most recent studies on the technology of nanocatalyst surface modification, including overcoming the internal and external constraints of nano catalysts and enhancing the process of photocatalytic destruction of innovative photocatalysts, and surface modifications [19]. Surface modification significantly improves the nano-ability catalyst's to catalyse reactions, which is advantageous for the degradation of innovative photocatalysts, and surface modifications. Low catalytic activity and unstable catalyst are just two of the drawbacks. New techniques for making catalysts should therefore be managed and given more focus in future research to enhance their overall performance. In the chosen mathematical setting, the probability links the two previous phases. The photocatalyst is the only factor that influences probability. It is unaffected by the quantity of the photocatalyst, the type of pollution, and the reaction's space-time.

Later, through experimental research, authors also underlined the

progress made so far in the photocatalytic capabilities of MOFs in energy and environmental remediation. Under the influence of sunshine, photocatalysis is utilized to use photocatalysts, nanomaterials, in a number of energy and environmental domains. This study focuses on the connection between the structure and functionality of photocatalysts because catalytic reactions occur on the surfaces of catalysts and because the interface structure of photocatalysts is crucial to the efficiency of charge carrier transfer. This includes a thorough discussion of the current issues, restrictions, suggestions, and opportunities. This exceptional study of the subject is concluded by sections on mechanistic considerations, computational modeling of photocatalysis, challenges and future outlooks of solar reactor strategy in engineering claims [20]. A special focus was on photocatalytic energy recovery, organic synthesis, and new reactor topologies, as well as the innovative characteristics of photocatalysis's applicability. Due to the noticeable causes of accessible reaction sites, surface management is essential in disciplines like gas sensors, photocatalysis, heterogeneous catalysis, and associated applications [21]. It seems even more essential when complex schemes are explored. In fact, several material characteristics are crucial in impelling the final qualities, including the catalyst habit (shape, and size which are closely associated to dangling bonds of active species), oxidation states of surface atoms, and surface oxygen vacancies (typically correlated with *in situ* generation of active intermediates, such as peroxides) [17]. These factors are between the most essential performers in the reactant transformation during the process under inquiry. It has in recent times been brought to light that traditional heterogeneous catalysis can give hints about surface changes [22]. Many important material classes in addition to metal oxide-based photocatalysts, such as innovative hybrid materials and carbon-based nanomaterials have examined [2]. Because of the extensive research on the photo-degradation of organic compounds, the ideal circumstances for this process heavily depend on the aforementioned variables. This review examines, in particular, how heterogeneous photocatalysis may be used to break down organic substances found in wastewater to provide an energy source like hydrogen or methane (Fig. 4).

The application of visible light-active photocatalysts and their effectiveness in the absence of noble metals have received particular attention [23]. The details of the experimental findings that support the idea of employing structured photocatalysts to simultaneously purify and valorize food industry wastewater are provided. It was also discussed in this review how photocatalysis is used to create organic molecule. Finally, we'll talk about novel reactor designs, like photocatalytic membrane reactors. An overview of the plasmonic metal's size, shape, geometry, loading, composition, and semiconductors' nano-structure and characteristics, of which are the primary factors influencing dye photo degradation, illustrated deeply. For photocatalytic applications, highly effective light-harvesting requires the creation of an appropriate structure with outstanding morphologies, interfacial structures, optical and surface properties, etc [24]. A thorough and relevant analysis of this significant and trending subject, with a focus on ecological claims and the possibilities for solar energy assembly. In plants and microorganisms, photocatalysis enables photosynthesis, and it also plays a key role in the chemistry of our planet's atmosphere (Fig. 5). The fundamentals of photocatalysis are thoroughly and methodically reviewed by covering topics including, kinetic modeling, reaction mechanisms, critical material characterization using cutting-edge methods, and new reactor design and scale-up [25].

Due to the extensive coordination between the active metal centres and the organic linkers, metal-organic frameworks (MOFs) are now regarded as novel photocatalysts [27]. Due to the huge surface area, organized structure, very porous nature, and extremely high structural tunability of this property, it offers special structural features. The historical evolution, synthesis, and alterations in MOF networks are all discussed in detail and critically in this review with reference to photocatalysis [28]. The current state of MOFs that are involved in photocatalytic activities such electron-hole pair creation, the formation of

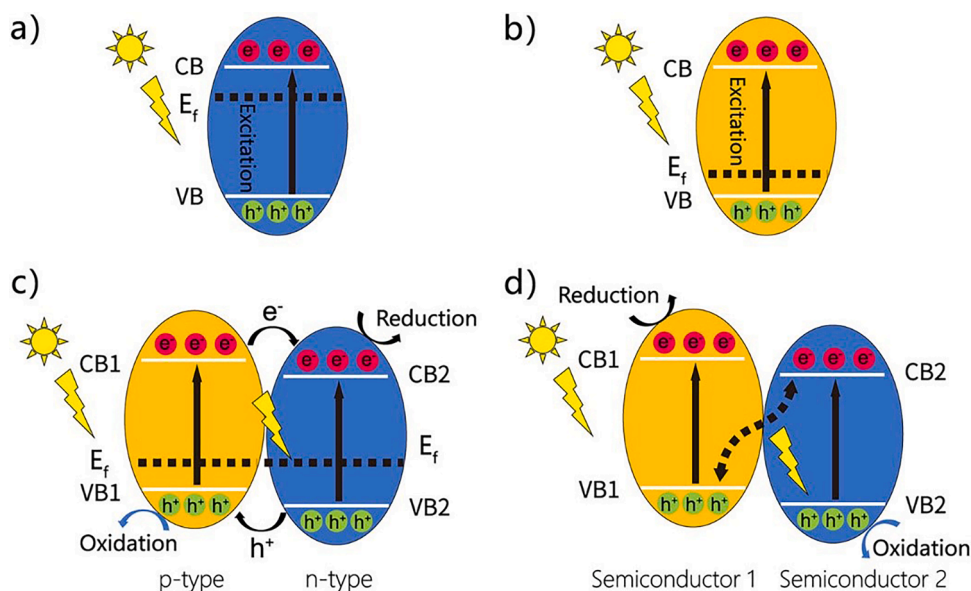


Fig. 4. A diagrammatic representation diagram showing the many kinds of photocatalysts, including single material photocatalysts (a) and (b), heterojunction photocatalysts (c), and (d) Z-scheme photocatalysts. Reprinted (adapted) with permission from Ref. [14]. Copyright (2016) Aleksandra B. Djurišić et al. APL Materials, AIP. Open Access under the terms of the Creative Commons CC-BY License.

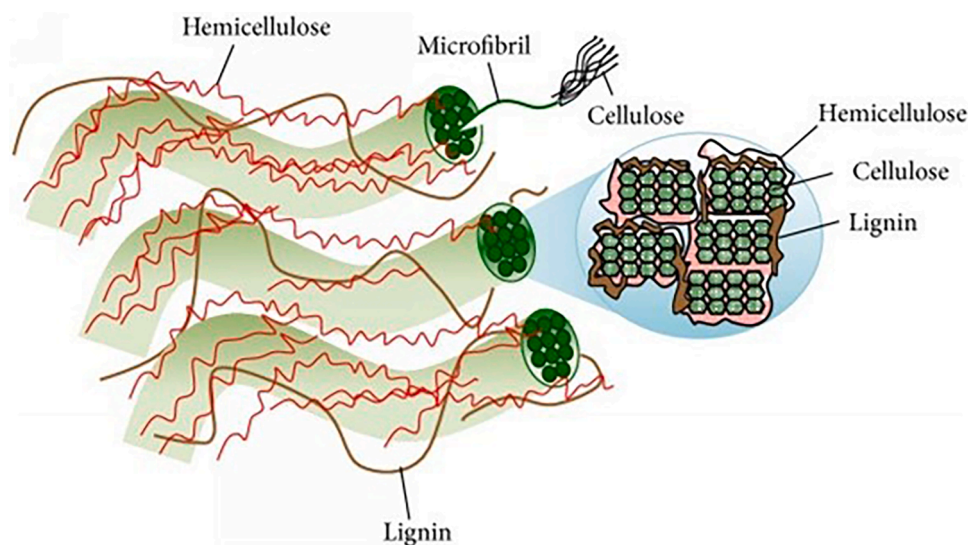


Fig. 5. An illustration of the cross section of a microfibril and the structure of a plant cell wall. Reprinted (adapted) with permission from Ref. [26]. Copyright (2014) H. V. Lee et al. Scientific World Journal, John Wiley & Sons, Inc. Open Access under the terms of the Creative Commons CC-BY License.

reactive species, and their impact on water chemistry have been discussed in detail. This study outlines a straightforward mechanism for forecasting how well phenol degradation will work in a photocatalytic device. The suggested scheme benefits from the sparing use of trial data and the absence of alteration variables that would force the scheme of equivalences to cover in the sagacity of the experimental statistics [29]. Using the Monte Carlo simulation, authors first determine the amount of energy absorbed over time and the amount of space that is exposed to radiation for the two types of photocatalysts that we have chosen. The next step is to identify a suitable theoretical kinetic model that can accurately depict how phenol breaks down into various intermediates and then CO_2 and water in the end. In our simulation, authors include a fresh consideration representing the likelihood that a photon immersed by the photocatalytic interruption performs its intended function, namely, to producing an oxidizing radical [30]. The developments and inventions in photocatalytic processes as well polymer photocatalysts

during the past few years are discussed. Recently, plasmonic photocatalysts have accelerated the improvement of photocatalytic performance under visible light radiation, boosting the possibility of harnessing sunbeams for eco-friendly and energy claims, including water splitting, CO_2 abatement, and wastewater handling [31]. A comprehensive overview and explanation on meaning of single-atom photocatalysts has delivered [32]. Formerly, a brief explanation of the metal-support interfaces on single-atom photocatalysts is specified. Following that, a summary of the single-atom photocatalyst characterization and methods currently used have also been added.

1.1. Photoelectrocatalytical reactions, and band-gap engineering

The study and replication of natural photosynthesis, arguably the most significant natural chemical activity, has resulted in huge growth in photocatalysis on semiconductor materials over the past two decades.

Water and carbon dioxide are transformed into oxygen and carbohydrates during photosynthesis, which uses solar energy. Similar to this, CO_2 and water can be converted into solar fuels via photocatalysis on semiconductor surfaces, which can also change water into oxygen and hydrogen. An in-depth knowledge of the fundamental physical concepts underlying the phenomenon of photocatalysis is necessary for the rational creation of new classes of photocatalytic materials. To achieve this, advanced and cutting-edge experimental procedures and theoretical approaches must be developed and used and illustrated in Fig. 6. A semiconductor nanoparticle's surface can be reached by electron-hole pairs produced by light, which can then trigger chemical processes such as chemical oxidation or chemical reduction. The primary necessity is to create semiconductors that enthrall in the visible spectrum and systems that lessen the occurrence of electron-hole recombination, but this effect significantly lowers the effectiveness of the photocatalytic conversion [33].

For describing the fundamental physical processes of photocatalysis, this section offers an overview of some of the most intriguing approaches and methodological developments. With time, new and diverse approaches have been used, including doping, composites, coupling, metallization, and dye sensitization [34]. For instance, surface and interface modification by the control of particle size and shape, doping of transition metal, doping of nonmetal, deposition of noble metal, composite or coupling materials, the application of co-doping (metal-metal, and nonmetal-nonmetal), use of organic dyes and metal complexes sensitizing surface, are all methods used to improve and increase the photocatalytic features [35]. It is possible to recruit a catalytic reaction because when dyes are wide-open to visible light, they introduce electrons into the semiconductors' conduction band (Fig. 7). The ideal circumstances to convert absorbed light directly into electrical energy with increased efficiency in solar cells or through hydrogen generation are a quick and fast electron injection and a sluggish backward reaction [36]. An unusual amount of interest in nanotechnology has generated the idea of adjusting the size and shape of semiconductor particles to boost their functionality and expand their potential applications. This idea is currently the subject of in-depth study. In addition to composition and structure, material properties are shown to be extremely sensitive to particle size and shape at the nanoscale. Along with its traditional functions in catalysis, control over the nanocrystals architecture has expanded the spectrum of semiconductor applications, allowing for developing light-emitting diodes, energy storage, medical diagnosis, and information processing [36]. Because of the crystallographic surface orientation, several metal oxide photocatalysts displayed significant differences in their photocatalytic activity.

(a) Photocatalytic features: Conceivable fundamental explanations

for the surface-dependent photocatalytic characteristics are examined from this angle. According to most of the data, varied surface happenings for photo-oxidation and photo-reduction processes are mostly caused by electron and hole diffusion toward various surfaces [38]. Either different band bending (or flat band potentials) occurs at the photocatalysts's interface with its surroundings, causing reversing charge transporter diffusion because of bulk anisotropies, or it results from flat band potentials [39]. Although the surface structure must be the primary cause of the surface electronic structure, no clear relationship between surface element and photochemical characteristics has been shown to date. The significance of surface charge separation and charge ensnaring at the exterior inspires fresh ideas for designing surface features with maybe higher photocatalytic activity [40]. Therefore, enhancements can be made by exposing surfaces to photocatalyst powders that have "naturally" higher photoactivity; optionally, the suggested method involves selectively modifying surfaces with specific surface phases or single layer heterostructures that enhance the electron transport at the surface [41]. Additionally, the bulk materials that would normally only be UV active may now be able to emit visible light thanks to specific surface phases with a decreased band gap. As the term "photocatalysis" has been used variously throughout the literature, which can lead to significant misunderstanding when not utilized carefully, our purpose in this section is to provide a comprehensive description of the term. The evolution of photocatalysis was, as will be seen in the section that follows, motivated by natural photosynthesis. From this vantage point, it should be acceptable to classify photocatalysis as a thermodynamically upward reaction. But the nature of the thermodynamic upward gradient itself can be a cause of confusion [42].

(b) Photocatalysis: Existed reactions do not occur spontaneously during the catalysis. A nonspontaneous reaction is therefore unanticipated to be made possible by the addition of a classical "catalyst." It is usual in the literature for authors to detect light as a reactant to resolve the terminology issues. This would change how the system's thermodynamics are viewed and allow the word "photocatalysis" to be applied broadly to such systems. The high activation energies of a wide number of spontaneous chemical reactions interfere with their dynamics [43]. Here, the reaction is made possible by the addition of light, which fits the traditional definition of catalysis. Therefore, photocatalysis is the most appropriate term to characterize these processes. The reactions that need externally applied potentials are another less visible class of reactions that frequently use the term "photocatalysis." They are referred to in the literature in a variety of ways, including photoelectrochemical and photoelectrocatalytic reactions (Fig. 8). In our opinion, whether it is photosynthesis or canonical photocatalysis, the basic processes engaged in these reactions are the same. Therefore, for the sake of

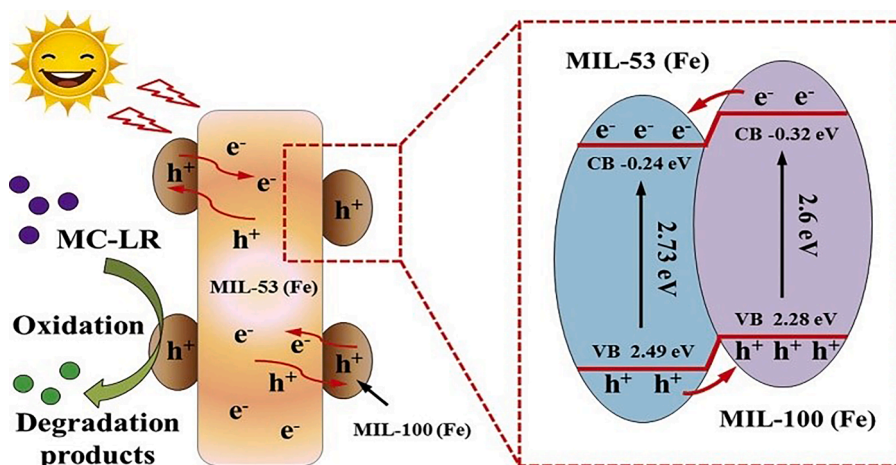


Fig. 6. A schematic illustration of photocatalyst mechanism. Reprinted (adapted) with permission from Ref. [24]. Copyright (2019) Yingping Huang et al. Applied Catalysis B: Environmental, Elsevier. Open Access under the terms of the Creative Commons CC-BY License.

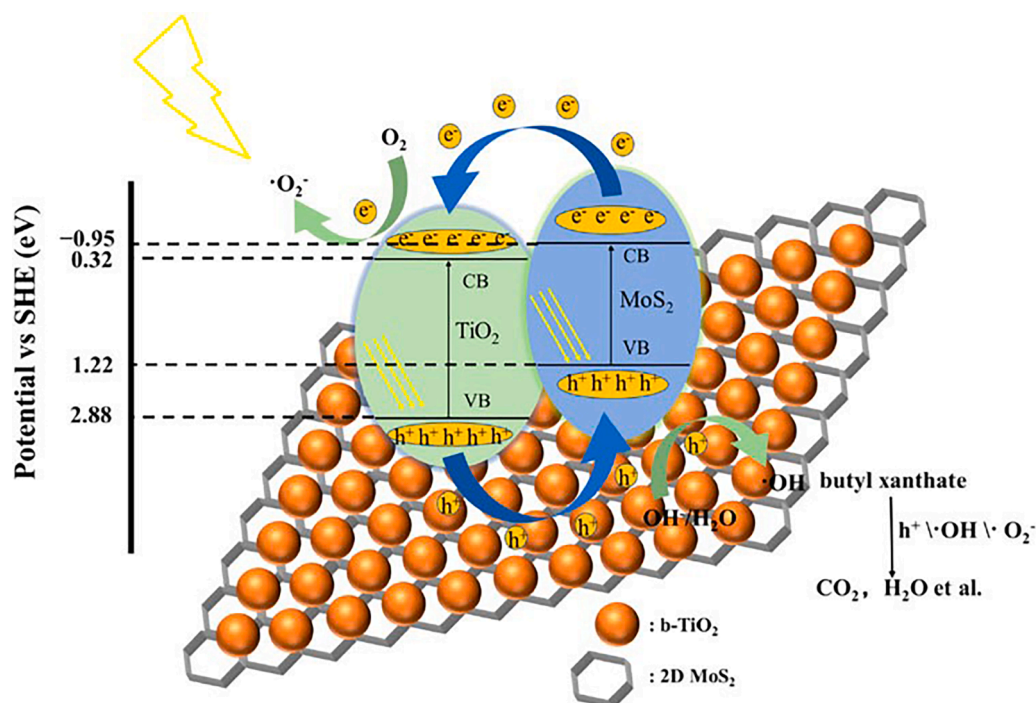


Fig. 7. A diagrammatic representation creation of $\text{TiO}_2@\text{MoS}_2$ heterostructures with increased photocatalytic activity. Reprinted (adapted) with permission from Ref. [37]. Copyright (2022) Haijun Tang et al. Colloids and Surfaces A: Physicochemical and Engineering Aspects, Elsevier. Open Access under the terms of the Creative Commons CC-BY License.

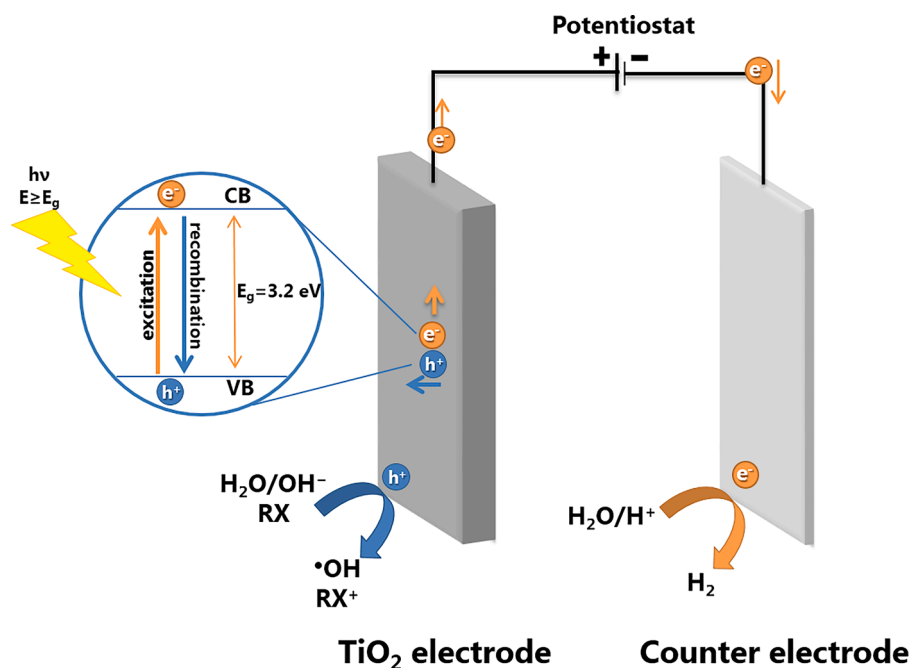


Fig. 8. The diagram shows the mechanism of charge separation in photoelectrochemical systems, which leads to a potential gradient, as well as the separation and recombination of charges in photocatalysis and photoelectrocatalysis. Reprinted (adapted) with permission from Ref. [45]. Copyright (2014) Maria Valnice Boldrin Zanoni et al. Modern Electrochemical Methods in Nano, Surface and Corrosion Science, IntechOpen Limited. Open Access under the terms of the Creative Commons CC-BY License.

comprehension and future growth, they ought to be viewed as a single group of responses [44].

Toxic pollutants, toxins, bacteria, and dangerous pigments are all frequently removed from the environment using photocatalysts. However, because of their greater bandgap, nanoscale semiconductors are often less effective than catalysts. Its efficiency can be raised by doping it

with the right substances, which will lower the material's bandgap and make the catalyst active in the visible spectrum [46]. This section primarily describes the reactions that the photogenerated electron-hole pairs take, as well as the underlying ideas and variables that influence the catalytic activity of the nanosized particles. Additionally, this unit allows the reader to adopt the numerous methods for improving the

photocatalytic characteristics of semiconducting materials by forming heterojunctions with semiconductor, metal, carbon, or multicomponent oxides. Since research on photocatalysis has a rather lengthy history, it is not essential to discuss its significance from a theoretical or practical standpoint [47]. For instance, the photocatalyst-coated window glass and outside walls have already attracted significant commercial interest due to their very advantageous ability to "self-clean," which permits the surface to be cleaned regularly however when exposed to light and rain [48]. In addition to these beneficial applications, the synthesis of hydrogen (H_2) from moisture by a photovoltaic radiation-induced photocatalytic activity is essential because it exemplifies a viable future technique for getting chemical energy from sources that are already plentiful, like water and solar light (Fig. 9a–c). Even when only solar photocatalysis studies are chosen, the findings of numerous scientific investigations on photocatalysis have been reported, making it seem fairly difficult, at least for the author, to conduct a thorough review by incorporating all or a significant portion of the reported studies on photocatalysis.

Of course, up-and-coming assessments have already published outstanding investigators on this subject. This section was not meant to provide a summary of all photocatalysis investigations published to

date, but rather to explain some of the essential concepts. In studies pertaining to photocatalysis, several of the characteristics have only been addressed as "common sense". The author has the pleasure of recommending reading reported the most recent assessment of the literature of researchers from worldwide on photocatalysis, which may be useful in comprehending the general framework of research on photocatalysis. Among chemical transformations, photocatalysis is a distinct class [52]. It makes use of the energy provided by light to propel challenging reactions, which are sometimes even impractical, to carry out in the dark. Photocatalysis has potential as a long-term solution for large-scale solar energy storage when applied to thermodynamically uphill reactions like photosynthesis. Current photocatalysis demonstrations are performed only in academic laboratory settings, despite the long-standing interest in this route and examination exertions [53]. One of the main causes of the slow advancement is the unavailability of appropriate photocatalyst substances for industrial claims [54].

(c) Photocatalytic materials: Numerous photocatalytic materials, charge separation techniques, and charge transfer methods, including novel photoelectronic materials and traditional semiconductors such as nanoscale plasmonic metal particles, 2D materials, and quantum dots, have all been investigated to achieve efficient light absorption. The 2D

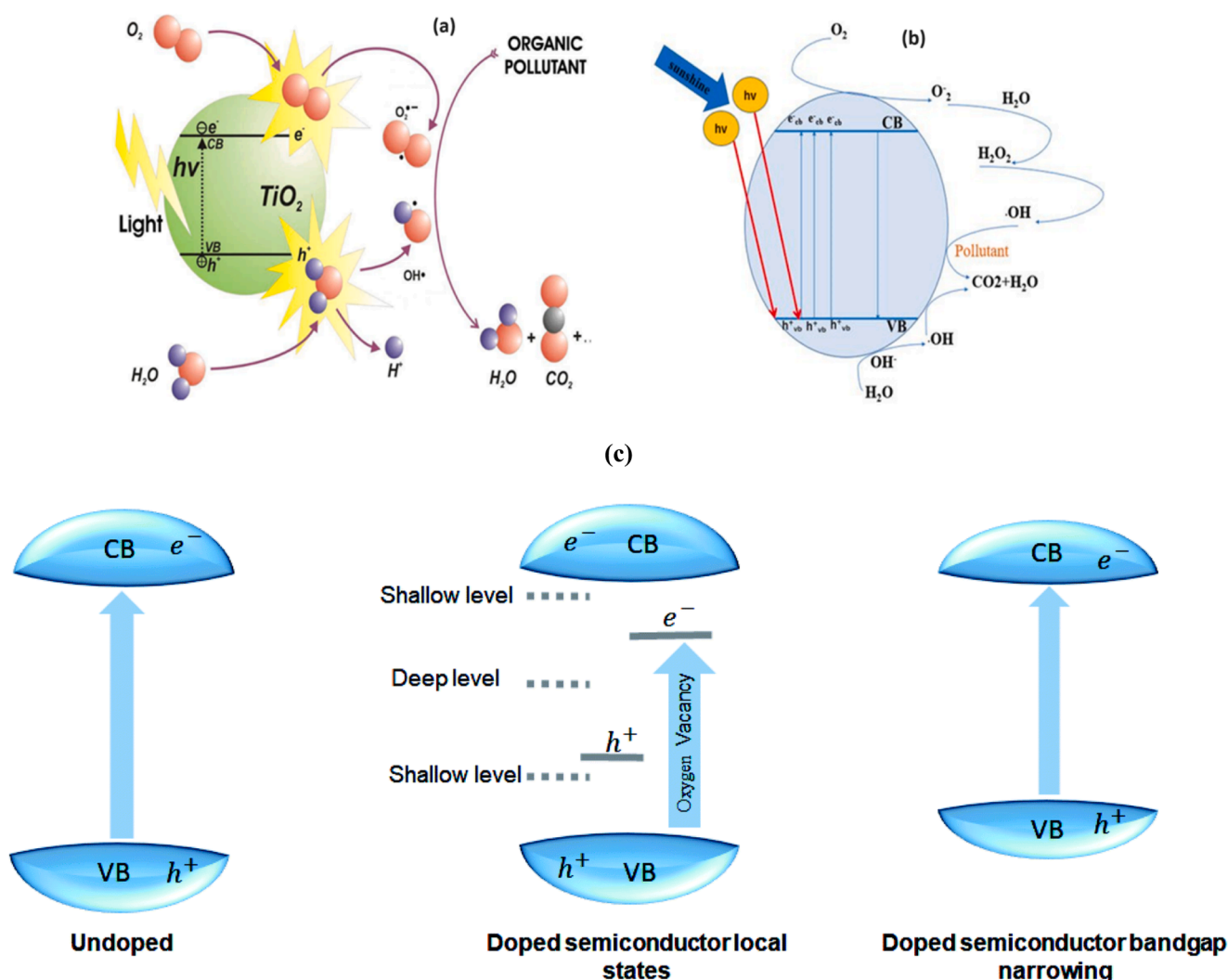


Fig. 9. (a). A schematic representation of semiconductor excitation by band gap illumination, which produces "holes" in the valance band and "electrons" in the conduction band [49]. Reprinted (adapted) with permission from Ref. [3]. Copyright (2013) Alex Omo Ibhaddon et al. Catalysts, MDPI. Fig. 9 (b). A schematic illustration photocatalytic reaction mechanism. Reprinted (adapted) with permission from Ref. [50]. Copyright (2019) Zhongyu Cai et al. Applied Sciences, MDPI. Fig. 9 (c). Doping's impact on bandgap. Reprinted (adapted) with permission from Ref. [51]. Copyright (2022) Muneeb Irshad et al. RSC Advances, Royal Society of Chemistry. Open Access under the terms of the Creative Commons CC-BY License.

materials exhibit numerous unique characteristics, including a great surface-to-volume ratio, an extraordinary degree of anisotropy, and programmable chemical activity [55]. Due to their use in photocatalytic systems, these special qualities of 2D materials have appealed an excessive planning of disquiet since they considerably expand light capture, surface reaction, and charge-transfer kinetics. This article introduces the advancements made in the study of 2D photocatalysts with various compositions and uses, followed by particular methods of surface modification. The systematically researched fundamental concepts in the 2D material-based photocatalytic systems include light harvesting, molecule adsorption/activation, and charge separation [56]. In the examples given below, 2D materials are used in a variety of photocatalytic energy-conversion systems, including those that produce hydrogen peroxide, synthesize organic compounds, reduce carbon dioxide, and fix nitrogen. This evaluation will deliver some creativeness for future research on 2D materials employed in effective photocatalytic energy conversion by describing the difficulties and potential solutions in generating these 2D materials [55]. The theme of this section is to provide a broad material perspective on these recent attempts, summarize them, and propose potential options for moving on to actual implementations.

The current energy crisis and environmental degradation are thought to be amenable to solution-using semiconductor photocatalysis [57]. One-dimensional (1D) nanomaterials have drawn excessive thoughtfulness in the realm of photocatalysis because of their distinctive architectures and exceptional physicochemical features. Nevertheless, they continue to face numerous challenges that have an adverse effect on their ability to perform as a photocatalyst in real-world settings, such as, quick recombination of low-apparent quantum efficiency, and photogenerated electron-hole pairs [57]. To address these difficulties, photocatalytic heterojunctions were built using 1D nanomaterials as the fundamental constituents and have shown distinctive and better-quality characteristics. The principles of photogenerated electron-hole pairs are used to evaluate a variety of heterojunctions based on 1D nanomaterials,

including type II heterojunction, Schottky junction, S-scheme heterojunction, Z-type heterojunction, and p-n type heterojunction (Fig. 10). The final section of the article discusses several difficulties and potential possibilities for 1D nanomaterial-based photocatalytic heterojunctions. The authors begin with an explanation of the fundamental concepts underpinning photocatalysis in general before analysing the many categories of photocatalytic materials and discussing a variety of aspects of their properties, such as reliability, affordability, durability, and scalability [5]. Then, to show the uses of these photocatalysts, authors simulate photocatalytic responses (water splitting, N_2 fixation, and CO_2 decline). The author offers our predictions for the future of the photocatalysis field at the conclusion.

1.2. Shaping photocatalysts: surface science of photocatalysis

The use of unrenewable energy sources, such as sunlight, to power activities on Earth has substantial obstacles, which photocatalysis promises to address. Scientists are becoming more and more interested in photocatalysis due to its potential advantages, especially its low cost and great efficiency compared to other processes. Emphasis is placed on the electrical and optical characteristics of photocatalysis while also discussing the theory and background needed to comprehend it. The examination of thermodynamics, photocatalytic principles, and kinetic factors, which affect the performance of the photocatalyst, comes next. Along with the difficulties of quantum proficiency, sensitivity to light, and photochemical firmness, the numerous kinds of accessible photocatalysts are conferred [58]. The basic principles, mechanism, benefits, and difficulties of photocatalysis are all covered in length in this section, along with how operational factors affect photocatalysis. The amazing process of photocatalysis has a wide range of uses, including the creation of hydrogen, air purification, antibiotic activity, and the photocatalytic destruction of numerous organic contaminants in wastewater [59]. Compared to other techniques, photocatalysis is rapidly developing and garnering greater interest due to its numerous advantages, such as its

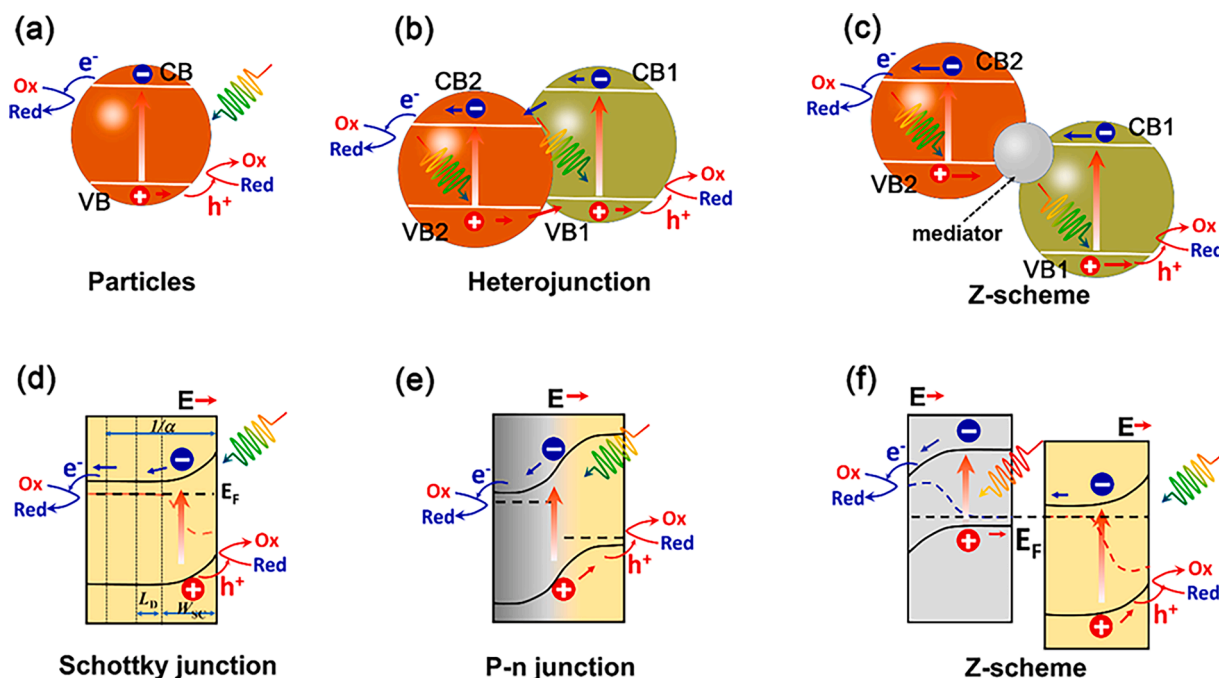


Fig. 10. Diagrammatic representation in semiconductor-based photocatalysis during charge separation; (a) charge separation. (b) Heterogeneous semiconductor particles in which CB1 and CB2 are connected via electron flow. (c) Z-scheme semiconductor particles that use electron mediators to assist the passage of electrons from CB1 to VB2. (d) When the Schottky junction (such as an n-type semiconductor) equilibrated with an electrolyte. To calculate light penetration, pace charge, and diffusion length, width, can be applied respectively. (e) Charge separation in a pn junction-equipped semiconductor. (f) Charge separation on p-type and n-type semiconductors. Reprinted (adapted) with permission from Ref. [2]. Copyright (2018) Dunwei Wang et al. ACS Applied Energy Materials, American Chemical Society. Open Access under the terms of the Creative Commons CC-BY License.

relatively inexpensive and potential effectiveness. Comparatively speaking, photocatalysis is growing swiftly due to its various advantages, including accessibility and alluring efficacy. Photocatalysis is a unique technique for addressing issues with energy and the environment (Fig. 11). Recombination releases the captured energy as light or heat (nonradiative recombination) (radiative recombination) [60]. The long-lived photogenerated charges on the surface may facilitate a variety of redox processes, the specifics of which will rely on the donor or acceptor characteristics of the species absorbed from the surface. Several exemplary approaches describing metal oxide- and chalcogenide-mediated photocatalytic reactions have been published, mostly concentrating on applications linked to energy and the environment [61].

The principles of photocatalytic activity and the surface characteristics of TiO_2 nanoparticles serve as the foundation for the authors' summary and discussion of the developments in the various surface modification techniques used up to this point [61]. These techniques include surface doping and sensitization, loading of nanoscale co-catalysts, exploiting surface F effects, and surface heterojunction formation, expanding the accessible surface areas, and exposing particularly reactive facets. Future attention should pay more attention to the fascinating synergistic effects of these numerous surface altering techniques [62]. Building incredibly effective TiO_2 and non- TiO_2

containing photocatalysts for organic photosynthesis, the manufacture of solar fuel, environmental cleanup, and other interconnected areas including solar cell fabricating, thermal catalysis, separation, and refining may be possible by examining these significant progresses in photocatalysis concepts, modifications, and surface features. Because it uses a powerful and environmentally sustainable energy source, photocatalytic NO_x treatment has recently congregated many concerns [63]. However, the majority of reported powdered photocatalysts are difficult to recover, and its use is restricted by the rapid rate at which poisonous NO_2 byproducts are produced. Here, a novel homogeneous protonated $\text{g-C}_3\text{N}_4/\text{graphene oxide}$ aerogel has developed by direct frozen-drying and discussed. Following the protonating process, a noticeable surface electrically charged change from the negative protonated $\text{g-C}_3\text{N}_4$ to the positive $\text{g-C}_3\text{N}_4$ is visible. The creation of electrostatic forces self-assembly to assist in the transfer of photo generated charge carriers ties this with negatively graphene oxide nanosheets [64]. With its plentiful porosity structure, improved visible-light absorption, and electron transport channel, graphene oxide aerogel serves as a monolithic substrate that enhances photocatalytic activity. It's significant to note that the addition of H atoms to the N atoms in $\text{p-C}_3\text{N}_4$ encourages oxygen atom activation, which enhances the oxidation of NO_2 to nitrate.

Recent research has provided unique, creative insights for

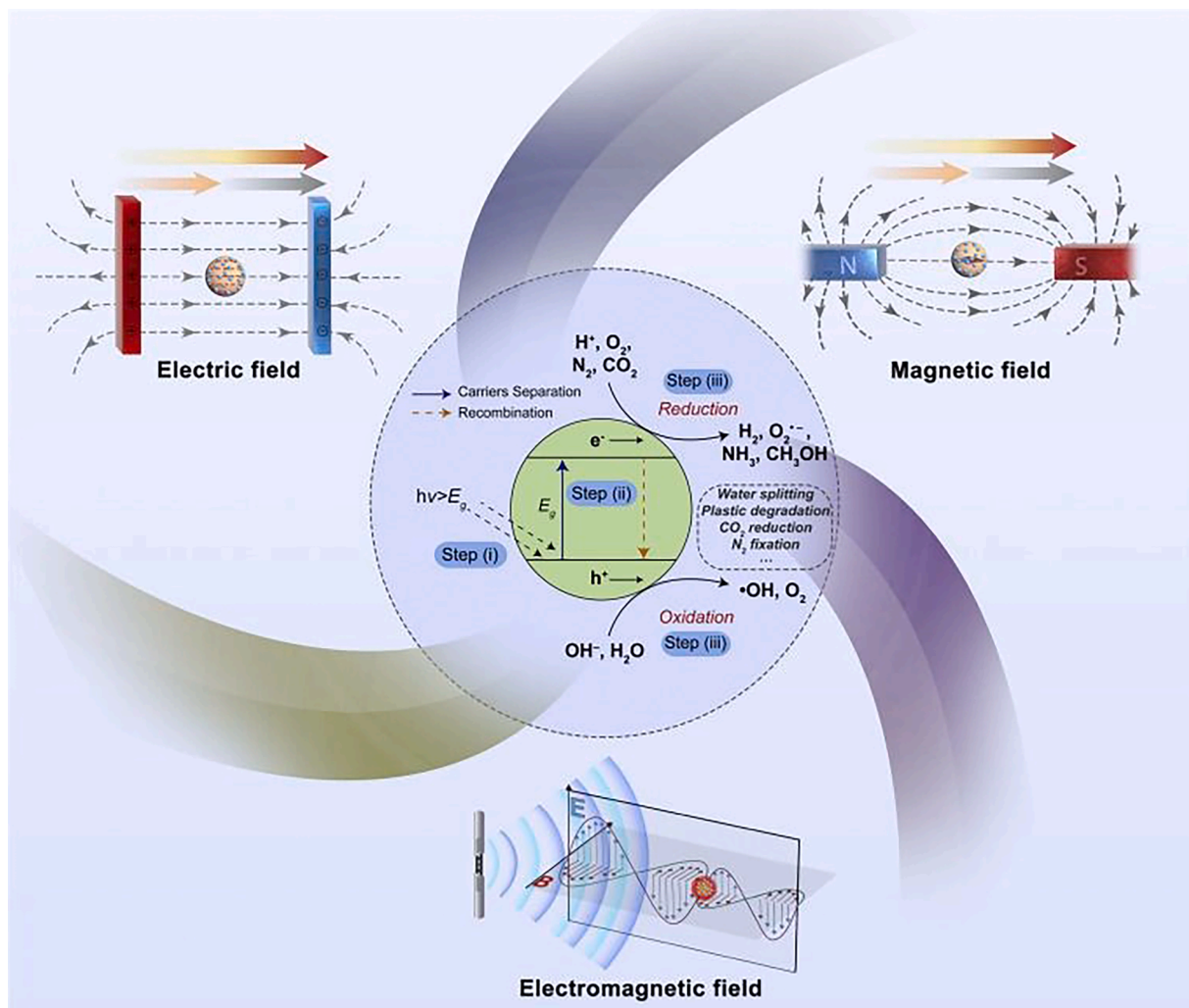


Fig. 11. A schematic illustration of various component of photocatalysis. Photocatalysis, aided by electric, electromagnetic and magnetic fields, involves surface chemical reactions, light absorption and charge carrier separation. Innovative catalysts with strong catalyst-support interactions can enhance local field effects, enhancing external field effects. Reprinted (adapted) with permission from Ref. [65]. Copyright (2022) Shik Chi Edman Tsang et al. Joule, Elsevier B.V. Open Access under the terms of the Creative Commons CC-BY License.

developing monolithic photocatalysts to regulate secondary pollutants for environmental cleanup. In the nonexistence of the liquid phase mass relocation restrictions imposed by aqueous suspensions, higher hydrogen production amounts were achieved with the photocatalysts in interaction with the vapor phase. The larger noble metal distribution on the photocatalyst surface is most likely the reason why the activity of photocatalysts containing metal nanoparticles was always greater comparatively photocatalysts made by deposition of proficient gold nanoparticles on TiO_2 . Octadecyl trichlorosilane (OTS) was used as a coupling agent to alter the surfaces of TiO_2 nanoparticles under various circumstances [66]. The grafting of OTS on the surface of TiO_2 nanoparticles was considered by thermogravimetric analysis and by other means. Fourier transform infrared techniques in order to enhance the nanoparticles' dispersion and to modify the interactions between nanoparticles under various situations has applied. The absorption of UV radiation with a wavelength between 200 and 900 nm was measured using an ultraviolet (UV) spectrophotometer. Rhodamine B was absorbed in the dark and destroyed under a lamp, and its absorbance was detected in UV/vis diffuse reflectance spectra to determine the catalytic activity of light [66]. The improvement of photocatalytic action has been accomplished with a practical approach that may also be used to modify other nanomaterials. Due to its capacity to address energy and environmental complications, heterogeneous photocatalysis using semiconductors were received a lot of interest as a sustainable and environmentally friendly technology in recent years. TiO_2 has been considered to be the best but also most thoroughly investigated photocatalyst among other semiconductors during the past ten years (Fig. 12).

(a) Surface modification approaches: Here, authors describe and explain the accomplishments of the numerous surface modification strategies applied to this point, including surface doping and sensitization, interface heterojunction formation, stowing of nano-sized co-catalysts, increasing the available surface regions, exploiting surface F effects, and exposing highly reactive facets. These techniques are all based on the essentials of photocatalysis as well as the surface composition of TiO_2 nanomaterials [67]. More focus in the near future should be paid, in particular, to the intriguing synergistic effects of these various surface alteration techniques. It may be possible to create extremely effective TiO_2 -containing and non- TiO_2 -containing photocatalysts for the production of solar energy, ecological cleanup,

carbon-based photosynthesis, and other connected disciplines including, thermal catalysis, solar cell device fabrication, separation, and purification by researching these significant developments in photocatalysis principles, surface chemistry, and modification. CO_2 is thought to be the most powerful and most common cause of global warming among all greenhouse gases. Concerning the current worldwide issue about industrial CO_2 emissions, photocatalysis is offered in this review as a viable technology [68]. To transform CO_2 into various high-value fuels, similar to methane, formic acid, methanol, and formaldehyde, photocatalysis uses a semiconductor material and sustainable solar energy underlined. In this section, the CO_2 reduction mechanism and routes are given along with a full discussion of the kinetic and thermodynamic codes of CO_2 photoreduction [69]. There are various techniques to improve CO_2 adsorption on semiconductor surfaces. TiO_2 , a semiconductor, is presently the subject of extensive research for its potential photocatalytic ability to reduce CO_2 when appropriately adjusted [70]. This is because of its effective photoactivity, high stability, low budget, and safety. The most modern techniques for synthesizing TiO_2 and altering it are discussed to increase the process' effectiveness in reducing CO_2 .

(b) Photocatalysis: In imperative to modify the TiO_2 light absorption, interfacial charge, and active surface as well as increase product yield and selectivity, these modification methods, which include semiconductor heterostructures, metal deposition, carbon-based material loading, metal/non-metal doping, and dispersion on high surface area support by including metal and non-metal doping. This section critically examines recent developments in CO_2 photoreduction using catalysts based on TiO_2 . In particular, the scenario where water is used as a reductant has led to an explanation of the photocatalytic mechanism of CO_2 reduction. There have also been compiled a number of techniques for altering TiO_2 , including deposition process, metal/non-metal doping, carbon-based material packing, semiconductor heterostructured creation, and dispersion on large surface area supports [71]. The potential surface modifications of TiO_2 photocatalysts have been discussed in a number of studies, but this study focuses on strategies that will specifically increase the CO_2 photoreduction efficiency of TiO_2 photocatalysts. Also mentioned are potential future avenues for effective CO_2 reduction by photocatalysis. Energy research has long struggled with the problem of creating artificial photosynthetic assemblies that

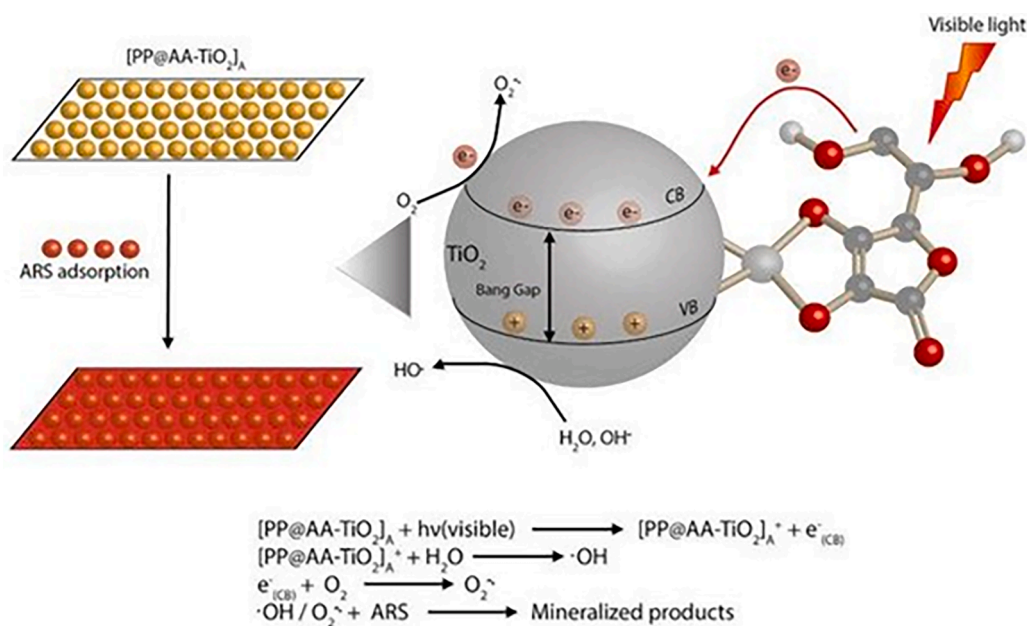


Fig. 12. Photocatalytic mechanism of metal oxide nano-photocatalysts towards photocatalytic degradation of chemical species. Reprinted from Ref. [4]. Copyright (2018) Chiara Anna D'Amato et al. Nanomaterials, MDPI. Open Access under the terms of the Creative Commons CC-BY License.

can operate under weak-intensity settings (like solar irradiation) and utilize the entire spectrum of visible light [72]. For achieving clean H_2 production from renewable resources on a large scale, semiconductor photocatalysis is a good source (Fig. 13).

Suppressing the rate of backward processes, including reverse electron transfer, is especially crucial for any artificial photosynthetic method where the normal Gibbs free energy change is positive. As an illustration, in Z-scheme overall water splitting with binary distinct photocatalysts and transportation of redox mediator, photogenerated electrons in the H_2 -evolving photocatalyst must be used by reducing H_2O (or protons) to H_2 while minimizing the reduction of more reducible electron-accepting species, which must be reduced by the O_2 -evolving photocatalyst [74]. The general study of photosynthesis, however, has wider implications than only solar energy storage, so it's vital to keep that in mind. It's fascinating in and of itself to think about how to power and/or enable chemical reactions using photon energy rather than heat [75]. Photocatalysis is the general term used in the literature to refer to this field of study. Providing a thorough overview of this topic is the aim of the review, authors are offering. The history of photocatalysis's evolution, its present state, and potential future prospects are all covered here. The reader will have the chance to concentrate on the significant common scientific benefits of seemingly disparate techniques because of our efforts to unify some sometimes muddled concepts surrounding the phrase "photocatalysis," which is the most essential goal of all [76]. The following categories best describe how the article is structured. Following an introduction to the historical perspective of photocatalysis, authors move on to discuss the fundamental principles that control photosynthesis. The following section provides a summary of the various photocatalytic reaction variations now in use [77].

Discussions on integrated systems, and featuring parts with various capabilities have presented and followed. After that, the study looks at how crucial interfaces between various parts of an integrated system. The authors offer their opinions on the direction the field is headed at the conclusion of the review. Moreover, this review focuses on the processes that occur on semiconductor-fluid interfaces when lit by light with the appropriate energy. Fundamental concepts, constraints, categorization, mechanism and operating conditions of photocatalytic reactions have explored in detail. Various photocatalytic processes' constraints, guiding principles, operational parameters, fundamental mechanism, and categorization are discussed with suitable references. In-depth discussions were also had regarding the most effective photocatalytic materials, their mechanism, problems they face, and how to fix

them [71]. Although the reactions and mechanisms involved in photocatalysis differ, the following four critical phases can be outlined: a photocatalyst surface can be charged in four different ways: (i) by absorbing light to create electron-hole pairs; (ii) by separating excited charges; (iii) by transferring electrons and holes there; and (iv) by using those charges for redox processes (Fig. 14).

A high percentage of electron-hole pairs recombine at the third stage, either on the surface site or while traveling there. The productivity and oxidation rates of photocatalytic systems are generally greatly influenced by a number of operational factors that control the photodegradation of organic molecules. Numerous published research findings have acknowledged how important these operational qualities are. The following are some fundamental elements that influence photodegradation: temperature of the reaction medium, solution pH, exposure time, substrate concentration, photocatalyst concentration, and other factors such as light intensity, the nature of the photocatalysts, the substrate, the oxygen content of the reaction fluid to be dissolved, ions of metal and non-metal doped, structure of the photocatalyst and substrate are depicted [79]. As an illustration, the work describes how produced heterostructured zinc oxide nanomaterials and lignin-based carbon photocatalyst were used to explore photodegraded routes (Fig. 15).

The same features are also examined when tetracycline degrades more quickly under visible light thanks to the TiO_2 nanotubes' greater surface area and more active sites with a smaller band gap (coupling of Cu_2O). On the photodegradation rate, the effects of several parameters including pH, photocatalyst loading concentration, tetracycline load, and cuprous oxide concentration, were examined [80]. Up to five successive batch cycles, the photodegradation effectiveness remains intact. The photodegradation of tetracycline is mostly mediated by superoxide and hydroxyl radicals, with valence band electrons being the least active reactive species, according to quenching tests [81]. Tetracycline's percentage of cytotoxicity and that of its degraded products both correlated negatively with that of their degradation. The photodegradation process' toxic-free effluent points to the potential applications of created photocatalyst in the sewage handling.

1.3. Mathematical modelling, probability and evaluation of photocatalytic degradation

Due to two aspects (i) the pioneers of the last century's intuition and (ii) the related improvement of scientists from various disciplines, including analytical chemistry, photochemistry, electrochemistry, radiochemistry, electronics, presumably catalysis, material chemistry and surface science, photocatalysis has currently emerged as a major field of study (Fig. 16) [82]. However, as heterogeneous photocatalysis is a subfield of catalysis, all the pillars of this field must be upheld. As a result, it is crucial to reframe the discussion of photocatalysis in order to eliminate contradictions and misunderstandings: (i) the response percentage is proportional to the mass of catalyst (low the plateau because of a full absorption of photons); (ii) thoughtful of compulsory application of the Langmuir-Hinshelwood mechanism for kinetics with the primary level is normally proportional to the coverages θ in the reactants; (iii) acquisition of conversions beyond the stoichiometric threshold means the number of potential active sites appeared on the surface at the beginning. An important phenomenon namely photonics must be considered along with photocatalytic action being (i) corresponding to the absorbance of the photocatalyst, and (ii) proportionate to the radiant flux Φ , support it to define the quantum yield, which is defined as the ratio of the reaction rate r in molecules (converted/second) with the efficient photonic flux (in photons / second) received by the solid material.

True photocatalytic standardized assessments should be developed to show actual catalytic action of illuminated materials, irrespective of non-catalytic lateral responses. The dye decolorization test, for example, is ambiguous since it solely assesses the dye's "visible" and apparent "disappearance," even though this process is purely photochemical and

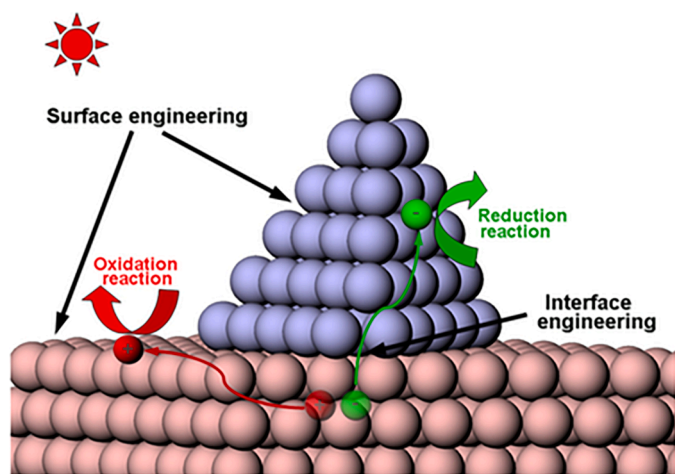


Fig. 13. Schematic representation of surface and interface engineering in photocatalysis. Reprinted (adapted) with permission from Ref. [73]. Copyright (2015) Yujie Xiong et al. Chem. Nano. Mat, John Wiley & Sons, Inc. Open Access under the terms of the Creative Commons CC-BY License.

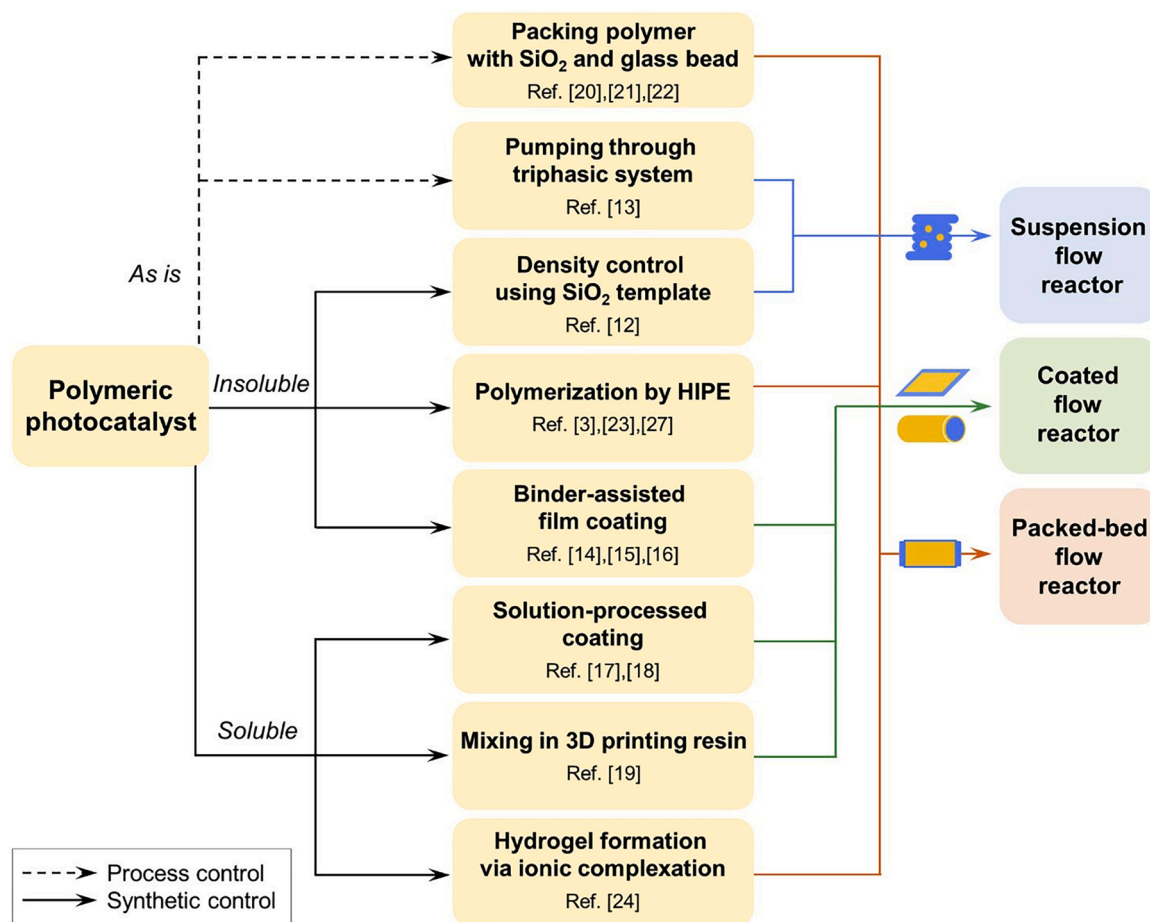


Fig. 14. Schematic representation of methods and artificial controls for adding polymeric photocatalysts to a flow photoreactor. Reprinted (adapted) with permission from Ref. [78]. Copyright (2022) Kai A.I. Zhang et al. Chem Catalysis, Elsevier B.V. Open Access under the terms of the Creative Commons CC-BY License.

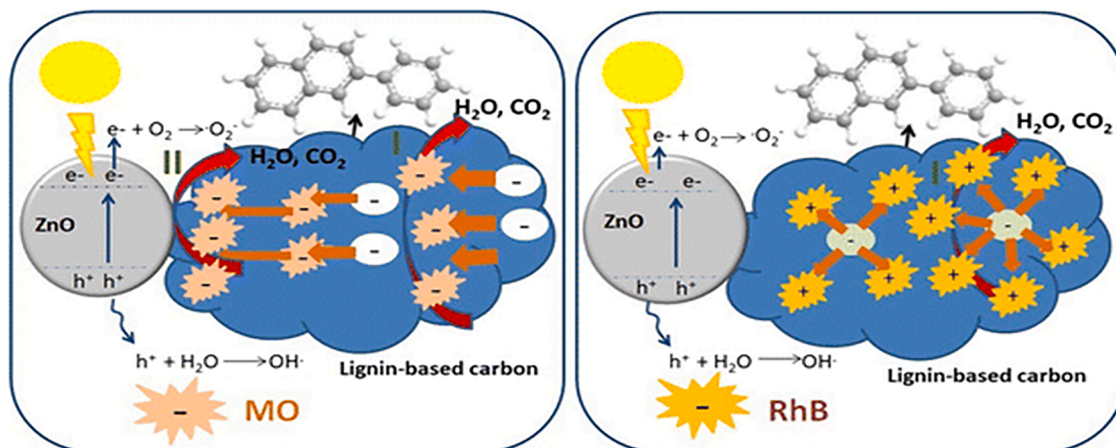


Fig. 15. A diagrammatic representation methyl orange (MO) and rhodamine B (Rh B) degradation over the LC-ZnO composite by a photocatalytic mechanism. Reprinted (adapted) with permission from Ref. [27] Copyright (2016) Roger Gläser et al. Topics in Current Chemistry, Springer. Open Access under the terms of the Creative Commons CC-BY License.

not photocatalytic [84]. Also important to consider is thermodynamics. In terms of thermodynamics, the production of highly active species like $OH^{\cdot}$ may be harmed by the reduction of photon energy to the visible spectrum [85]. Cationic doping is now officially acknowledged to be harmful for photocatalysis in solid state chemistry [86]. Anionic doping needs to be quickly explained or stopped altogether. In conclusion, each of these suggestions must be taken into consideration and studies must

be conducted under appropriate conditions before it can be said that one is dealing with a true photocatalytic reaction, the authenticity of which may be established by adhering to the methodology provided at the end.

(a) Mathematical modelling: The mathematical model was developed in light of the fact that the catalytic oxidation of MB, (R), which was expressed mathematically by the equation, occurs mostly during illumination of white LEDs; as $V \cdot \frac{dC(t)}{dt} = r(C, I) \cdot W_{TD}$; where where V is

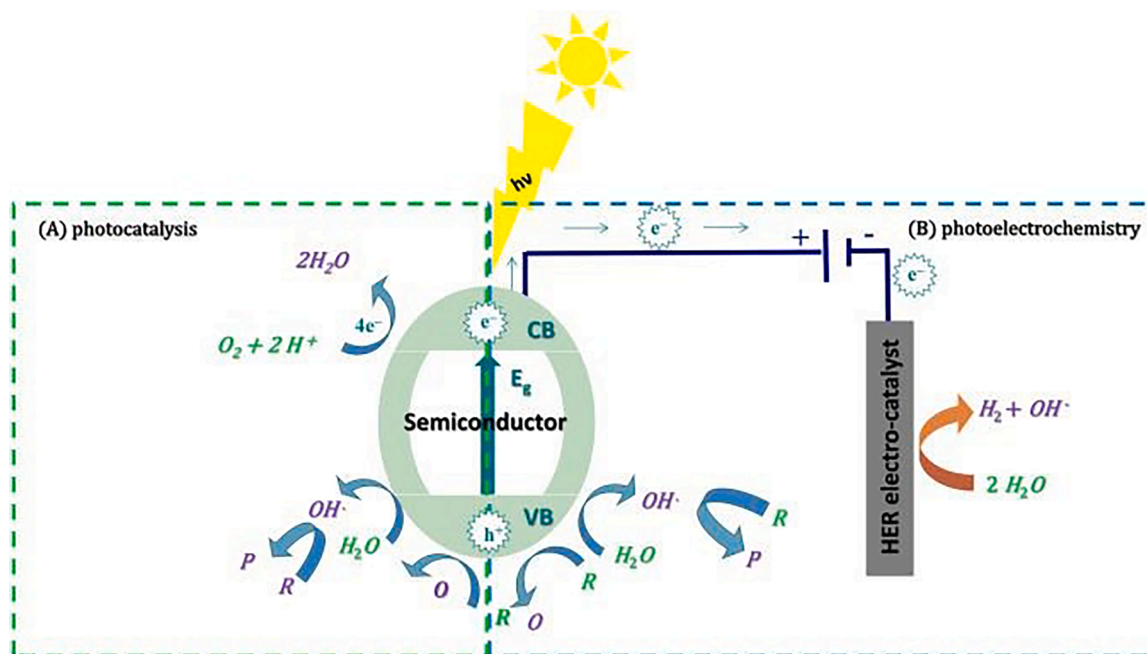


Fig. 16. A diagram of (a) photocatalysis and (b) photoelectrochemistry processes. Reprinted (adapted) with permission from Ref. [83]. Copyright (2020) Ronald Vargas et al. Energy Reports, Elsevier B.V. Open Access under the terms of the Creative Commons CC-BY License.

the solution volume (L), $C_1(t)$ is the MB concentration (mg / L), $-r$ is the reaction rate (g / L. min), W_{TD} is the catalyst quantity (g), I is the light intensity approached photo catalyst surface (mW/ cm²) [87]. Consider the primary settings as; $t = 0$, $C = C_{in}$.

The following possibilities for kinetic terms are included in the model:

(a). $-r = k_1 \cdot f_C \cdot g_1$.

(b). $f_C = \frac{b \cdot C}{1 + b \cdot C}$, this expression is the like the Langmuir–Hinshelwood rate law applied earlier [1]. (c). $g_1 = \frac{a \cdot I}{1 + a \cdot I}$, a straightforward method [88]. for designing photocatalytic reactors was also documented in literature, taking into account that photons are the outputs of inconsequential constituents [89].

This statement confirmed the existence of the photocatalyst particle only absorbs a small portion of the light that reaches it. The parameter was used to assess this effect. However, it is crucial to keep in mind that while the light infiltration diminutions with the amount of the catalyst during interruption because of the screening effect, the availability of active sites rises [90]. This implies that the photocatalyst particles will only get a small amount of the luminosity entering the reactor.

1.4. The Monte Carlo simulation

In general, the Monte Carlo simulations define a method of computation that uses many random samples to obtain results. They are often used in physical and mathematical problems and are most useful when it is difficult or impossible to use other mathematical methods. Monte Carlo methods are mainly used in three distinct problem classes namely - optimization, numerical integration, and generating draws from probability distributions. The following steps in the mathematical procedure of Monte Carlo simulation are necessary to calculate the LVRPA, and they are as follows:

- [1] **The photons wavelength:** The UV light source's emission spectrum will be used to determine the winners of a random drawing [91]. The outline of the emission bend of the lamp $D(\lambda)$ is measured as bell arch or Gaussian curve, where $290 < \lambda < 410$ nm, an probability of 370 nm, and a difference of approx. 40 nm² value [91]. Therefore, the distribution will be followed to make

the wavelength draw: $\text{Dis}(\lambda) = \frac{D(\lambda)}{\int_{290}^{400} D(\lambda) D\lambda}$, where

$\int_{290}^{400} D(\lambda) D\lambda$ is the matching the total amount of photons injected during the simulation [91].

- [2] **The photon positions on the light source:** It is presumptively true that the lamp's UV emission adheres to the Extended Source with Superficial Emission (ESSE) [92] model, which depicts a uniform emission from the lamp's surface freely [91]. Every photon has a initiation centre in the light initiator, which is, as was previously revealed, a cylinder with a radius, $R_L = 0.75$ cm and a height $h_R = 24$ cm [91]. Spherical coordinates are used to express the photon positions, (x, y, z) : $x(i) = R_L \cos(\gamma(i))$, $y(i) = 2\pi \zeta_1(i)$; $y(i) = R_L \sin(\gamma(i))$; $z(i) = h_R \zeta_2(i)$; where $\zeta_x(i)$ are arbitrary statistics uniformly defined from the intermission [0, 1]. Each photon i selected based on its wavelength i and initial location (x, y, z) on the lamp i will advance by a small opening step until it reaches interior section of reactor [91]. The only restriction placed on the photon's initial extent is that there must not be a first-movement crash with the light creator [91]. The coordinates (x, y, z) of the photon (i) will be observed by: $x(i) = R_L \cos(\gamma(i)) + s(0) \cos(\theta(i)) \cos(\delta(i))$; $y(i) = R_L \sin(\gamma(i)) + s(0) \cos(\theta(i)) \cos(\delta(i))$; $z(i) = h_R \zeta_2(i) + s(0) \sin(\delta(i))$ with, $\theta(i) = \gamma(i) - \frac{\pi}{2} + \pi \zeta_3(i)$; and $\delta(i) = -\frac{\pi}{2} + \pi \zeta_4(i)$. where each sign and notation is used in accordance with its usual interpretation.

- [3] **Photon transition, situations and the reaction volume:** The wavelength affects the likelihood that a photon will transition in the area that has been exposed to radiation. If higher is the wavelength $\lambda(i)$, then higher is the transmittance $T(\lambda(i))$. Therefore, if the photon's energy quantum is low, it has a higher chance of slipping past the inner tube's wall [91]. Corresponding to each $\lambda(i)$, $T(i)$ will be considered as per mathematical expressions: $\lambda < 290$; $T(\lambda) = 0\%$; $290 < \lambda < 340$; $T(\lambda) = 0.0184 \lambda - 5.336$; $\lambda > 340$; $T(V) = 92\%$ [91]. A random number $\zeta_5(i)$ will be drawn. If it is less than $T(i)$, the photon will be transferred to the illuminated capacity [91]. If not, it will be immersed and the photon $(i + 1)$ will be reflected.

- [4] **Optical properties measurement and moving step of suspension:** Calculations are made regarding the optical characteristics that rely on wavelength when the photon I passes through the suspension: $\sigma_i(i)$ and $k_i(i)$ are correspondingly the definite scattering and particular absorption coefficient, and interconnected as $\beta_i(i) = \sigma_i(i) + k_i(i)$ is the specific extinction coefficient; and $\omega_i(i) = \frac{\sigma_i(i)}{\beta_i(i)}$ is the albedo of the photocatalyst (Fig. 17) [91]. The distance between two occurrences is measured by the photon's travelling stride [91]

The Beer–Lambert–Bouguer law, defines light attenuation by scattering and absorption at two points x_1 and x_2 , can be

$$- \int_{x_1}^{x_2} k_t(x) dx$$

expressed by the mathematical expression $e^{\int_{x_1}^{x_2} k_t(x) dx} \leq 1$, where k_t is the volumetric extinction constant in the considered medium [91]. It is expressed as the sum of the volumetric scattering and absorption constants as $k_t(\lambda(i)) = k_d(\lambda(i)) + k_a(\lambda(i)) = (C_{TiO_2}) \beta_i(i)$. Where C_{TiO_2} signify the mass concentration of the particles participate in the medium. k_t , therefore, based on the photocatalyst's quantity and photon's wavelength [91].

- [5] **Selecting the category of event:** The albedo (x), which is the capacity of the photocatalyst to reflect light, influences the kind of event that occurs at each movement step of the photon in suspension [91,93]. The possibility of scattering at the surface increases as albedo increases C_{TiO_2} . The albedo is subjected to the wavelength of the photon and on the nature of the C_{TiO_2} [91,93] each photon, chosen at random using the aforementioned Gaussian distribution and re-counting the lamp's emission spectrum, [94] has its albedo value as specified in the expressions, $\omega(\lambda)_{p25} = 0.00491 \lambda - 1.115$, and $\omega(\lambda)_{UV100} = 0.00454 \lambda - 1.007$. If $\gamma_7(i)$ if the photon's albedo I is greater than the value, the photon will be absorbed [94,93]. To determine the absorbed energy, the absorbed photon's position and wavelength will be noted [91]. In the absence of this, the photon will be discharged, and the phase function will decide its new coordinates, $p(\lambda(i))$ [91]. The diffusion regime affects how the phase function is expressed (regime of Mie scattering or Rayleigh).

- [6] **The determination of the native volumetric rate of photons immersed (LVRPA):** Based on the radii, the irradiated volume was separated into 20 distinct volumes, R_{ext} and R_{int} of the tubular reactor [91]. Hence, the k th volume will be: $V_R^k = \pi h_R \left[\left\{ R_{int} + k \left(\frac{R_{ext} - R_{int}}{20} \right) \right\}^2 - \left\{ R_{int} + (k-1) \left(\frac{R_{ext} - R_{int}}{20} \right) \right\}^2 \right]$. [91].

Every absorbed photon will have its position recorded and its matching volume calculated [91]. The LVRPA of the k th volume

will be given by the expression, $LVRPA_k = \frac{n_{photons}^{absorbed(k)}}{V_R^k}$.

(b) MC simulation and outputs: The irradiated area of the photocatalytic device absorbs light more effectively when the photocatalyst load is increased. In fact, according to mathematics, increasing the photocatalyst load causes the volumetric extinction coefficient to rise, (k_t) [$\ln k_t(\lambda(i)) = k_d(\lambda(i)) + k_a(\lambda(i)) = (C_{TiO_2}) \beta_i(i)$], this causes the photon travelling step to be reduced in $s(i) = -\frac{\ln(1-s_0(i))}{k_t}$, and hence a rise in the quantity of photon absorption instances in our simulations [91]. Although there has been an improvement in total light absorption, the near stasis or fall in photoactivity could be explained by an increase in the dead volume corresponding to the load of TiO_2 . In keeping with this line of reasoning, we added a fresh idea to our kinetic model: the correction coefficient of the irradiation volume, $C_f = \frac{V_{vac}}{V_R}$, the to the volume consumed in the storage tank, our model will add dead volume, and we have $V_{Bf} = V_B + (1 - C_f) V_R$, with $V_B = 594 \text{ cm}^3$, the volume of air being circulated before correction [91].

1.5. Reconsidering the definition of photocatalysis: energy bands and levels

In photochemical reactions, there are, as we all know, two laws [95]. In the first, it is stated that only light that a substance absorbs can result in photochemical reactions, and in the second, the renowned photoelectric effect equation is used [96]. They both suggest that a photon is a particle of energy that enters the reaction system [97]. Some theories, however, held that photons may serve as reactants in physicochemical processes [98]. With the help of an analogy with the electrochemical process, a revised description of photocatalysis is suggested based on this understanding. We describe the suspended photocatalytic systems by illustrating photocatalytic water splitting in the acidic electrolyte. The valence band electrons are excited to move into the conduction band by monochromatic photons with frequency (ν). The excited electrons are then transferred to the surface and reduced the H_2O . The H_2O electrons are moved to the valence band, which has a lower electron energy level. Thus, the reaction routes defined as: $h\nu + e^- (V) \rightarrow e^- (C)$; $2H^+ + 2e^- (C) \rightarrow H_2$; $H_2O \rightarrow 2H^+ + \frac{1}{2}O_2 + 2e^- (V)$, where all symbols and notations are having their usual meanings. It is commonly accepted that photons have a chemical potential of 0, which enables electromagnetic waves of various frequencies, orientations, and intensities to coexist steadily in the same "phase" without undergoing mutual photon energy conversion [99]. The photocatalyst maintains the reaction equilibrium, just like electrocatalytic water splitting does [100]. Since photons are the reactants in all light-induced catalytic processes, regardless of how much the free energy of chemical reactions changes, photocatalysis is the general term for all such processes.

A band diagram is often used to show the electrochemical composition of a semiconductor material. It plots the energy bands and energy levels against position. The energy levels in the VB and CB of a semiconductor are basically continuous in terms of the vertical energy scaling and the horizontal spatial dimension [101]. EVB stands for the upper edge of the valence band, whereas EB stands for the lower edge of the conduction band and denoted by E_{CB} . The Fermi level is found inside the band gap, and Fermi energy is equivalent to the semiconductor's electrochemical potential ($E_F = \mu_e$) [101]. The work function of the semiconductor is given by the mathematical expression $\Phi_{SC} = -\mu_e - e\psi$ where all symbols and notations are having their usual meaning [101]. The work function shows the amount of effort required to drive an electron x distances away from a solid surface, where the classical images-force potential ($-\frac{e^2}{4x}$) is just negligible. In general, 10^{-4} cm distance is adequate to meet such necessity [101].

1.6. Analogy analysis of electro catalytic water splitting

There are several so-called non-spontaneous ($\Delta G > 0$) reactions for electro catalytic processes, with the electrolysis of water serving as one common example and denoted as $H_2O \rightarrow H_2 + 1/2O_2$, $\Delta G_0 > 0$. This process should be described as "electrosynthesis" as opposed to "electrocatalysis" in accordance with the definitions of the two terms, photocatalysis and photosynthesis. Researchers in electrochemistry have suggested the idea of electrochemical potential to circumvent this issue, (Ψ_i^α) [95]. For species i with charge z_i in α phase, we have a mathematical expression as, $\Psi_i^\alpha = \mu_i^\alpha + z_i F \phi^\alpha$. Where all symbols and notations are having their standard meanings. To assess whether a reaction can occur spontaneously, the electrochemical free energy ($G1$) rather than the free energy ($G2$) is utilized as a criterion. It also maintains the essential link with the electro-chemical potential. For the electrons in α phase, the Ψ_i^α is given by the expression, $\Psi_i^\alpha = \mu_i^\alpha - F \phi^\alpha$ [95]. To guarantee that the chemical potentials of electrons at both electrodes are same in vacuum, the anode and cathode of the electrolytic cell for electrolytic water splitting are two identical Pt electrodes ((given as Pt_A anode and Pt_C cathode), to guarantee that, in vacuum, the chemical potentials of electrons at both electrodes are the same. The electrolyte is believed to

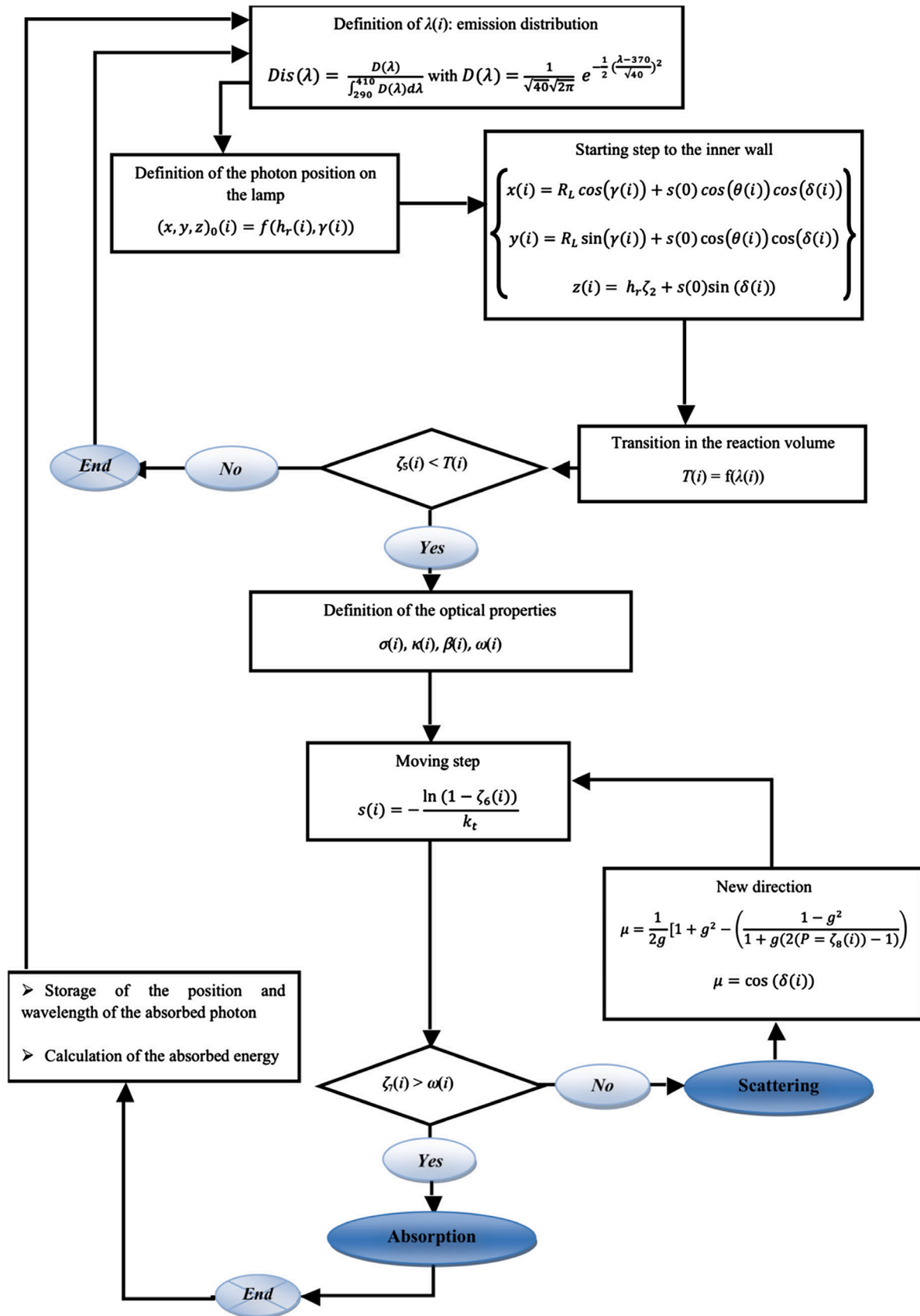


Fig. 17. Schematic illustration flowchart of M-C simulation in suspension mode [91]. Reprinted (adapted) with permission from Ref. [91]. Copyright (2013) Christophe Colbeau-Justin et al. Chemical Engineering Journal, Elsevier. Open Access under the terms of the Creative Commons CC-BY License.

be in an acidic environment, and a bias Vapp is placed between the two electrodes [95,102,103]. At the anode, H₂O is oxidized and electrons are transferred to the Pt_A: $\text{H}_2\text{O} \rightarrow 2\text{H}^+ + \frac{1}{2}\text{O}_2 + 2\text{e}^- (\text{Pt}_\text{A})$. Also at the cathode, H⁺ is reduced by the electrons such as $2\text{H}^+ + 2\text{e}^- (\text{Pt}_\text{C}) \rightarrow \text{H}_2$. The electro catalyst performs the same function as other catalytic systems in this process, except kinetically accelerating rather than having a thermodynamic impact on the electrocatalytic process [104]. Simply expressed, the equilibrium of the reaction is unaffected by the electro catalyst.

1.7. Emerging scientific opportunities: surface engineering and interface modification in photocatalysis

Over the past few decades, the photocatalysis, which directly converts solar light into chemical energy, has drawn a lot of attention as a potential remedy for the global energy issue and environmental pollution. To apply "photocatalysis" in commercial and daily life, it is necessary to develop photocatalysts that have good selectivity, stability, steadily and high activity, as well as recognized. Advanced materials with well-defined sizes, forms, architectures with desired arrangements that were innovated comprehensively as photocatalysts for numerous applications, including water splitting, pollutant degradation, (Fig. 18) and CO₂ reduction, to achieve this titled objective [105]. Particularly, size shrinkage increases the quantity of catalytic sites and may also customize the electrical structures at the micro- or nanoscale. This significance of surface responses is typically certified together complex and hybrid structures. The interface between two neighboring constituents in hybrid structures, where charge carriers are transmitted, is a further critical feature. The routine of charge transfer across several light-harvesting centres and from one light-harvesting constituent to reaction locations influences the structure and quality of interfaces [106]. To entirely functionalize the multi-component material structures, the interface and surface assemblies must be thoroughly controlled. While creating photocatalytic materials, it can be challenging to engineer at the interface and surface sites. It is important to make a few crucial interpretations regarding the facet-engineered surface and interface design before moving on to the debate of monitors. The persistence of this facet production is to improve photocatalytic routine by logically altering the surface and interface architectures of

photocatalysts [106].

In recent studies, other photocatalytic material featured, including as chemical arrangements and crystal assemblies, should be held persistent accurately to reflect the connection between facets and photocatalytic routine. Due to, it is necessary to apply sophisticated synthetic protocols with great parameter controllability to prevent other parameter variations from interfering with the results of facets-dependent research. As just the surface of the light-harvesting constituent needs surface adjustment, the surface engineering of mono-component photocatalytic materials is quite straightforward [107]. In contrast, because numerous constituents are involved, there are more surfaces and interfaces form between the components, making facet engineering on photocatalytic hybrid systems far more demanding. Note that in some hybrid photocatalysts, specific surfaces do not operate as the energetic locations for catalysis and definite interfaces do not function as conduits for charge carrier transit (Fig. 19). Their facet adjustment is rendered ineffective in modifying the charge kinetics and refining the photocatalytic performance due to these possibilities [108].

(a) Facet engineering: The sensible design of appropriate surfaces and interfaces is thus a crucial aspect of facet engineering. It is important to take the structural correlation between the surface and the interface into account when changing the surface of a hybrid construction. The interfacial structure, for instance, will be inherited from the surface facet of the component when an interface is assembled on its surface. Consequently, altering an existing component's exposed facet will necessarily cause changes to the interface's facet structure. The well-stated parameters deliver a framework for comprehending how they relate to the photocatalytic routine and enable control of the performance through parameter tweaking [110]. Through the creation and transfer of charge transporters, safety kinetics plays a crucial role in the conversion of solar energy into chemical energy during a typical photocatalytic process. In terms of charge kinetics, a process of this complexity consists of three fundamental phases: (a) charge creation under semiconductor light stimulation; (b) charge transfer to the catalyst surface; and (c) on the catalyst surface, redox processes consume charge. The effectiveness of each phase shows a noteworthy role in how well a photocatalyst work overall. To optimize solar-to-chemical energy alteration, it is crucial to streamline and harmonize the events. Overall,

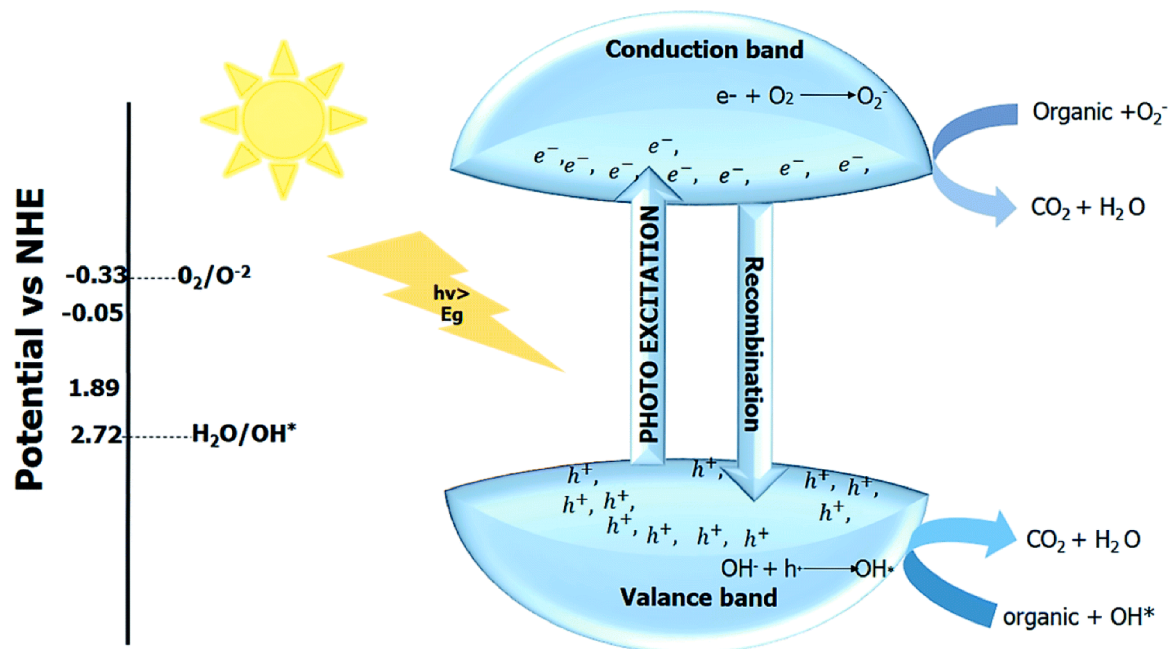


Fig. 18. An illustration of degradation of pollutants via photocatalysis. Reprinted (adapted) with permission from Ref. [51]. Copyright (2022) Muneeb Irshad et al. RSC Advances, Royal Society of Chemistry. Open Access under the terms of the Creative Commons CC-BY License.

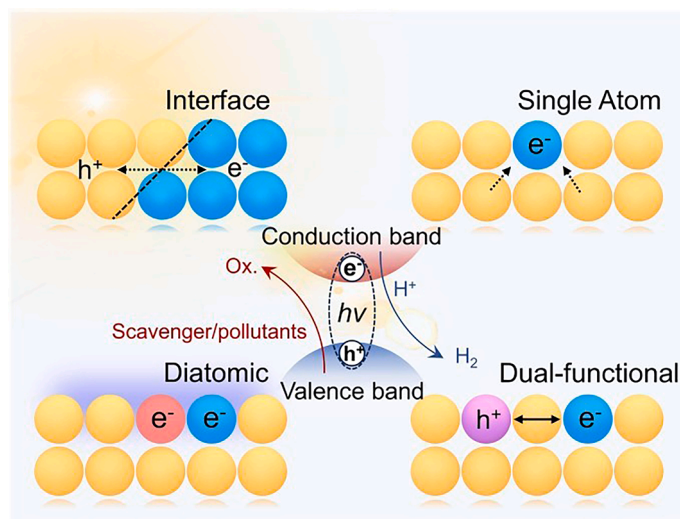


Fig. 19. A diagrammatic highlighting surface and interface structures of photocatalysts. Reprinted (adapted) with permission from Ref. [109]. Copyright (2024) Sihui Zhan et al. Science China Chemistry, Springer Nature.

to achieve it, photocatalytic materials recently underwent an evolution from simple semiconductors to multi-component composite architectures. In past, it has been demonstrated that the synergism of the various components in hybrid photocatalysts can revive the light absorption variety for charge generation, diminishing electron-hole recombination for charge transfer, or advance reactant adsorption and initiation for charge feasting [111]. Because the synergism depends on the hybrid photocatalysts's surface and interface designs, it holds out hope for improving photocatalytic performance [112]. The effectiveness of reaction molecules accepting photogenerated charges toward the invention assembly is significantly inclined by the surface where the redox reactions transpire. The facets that make up on the surface and interface

are the crucial variables that must be properly designated in order to govern the interface and surface structures (Fig. 20).

The facets exposed on the surface of the photocatalyst may affect the photocatalytic action through a variety of distinct operational mechanisms [114]. For example, the selectivity of surface electronic band structures (i.e., surface states) prevents the adsorption and activation of reaction molecules. By altering the catalytic performance, which depends on surface facets, photoinduced charge carriers would be given customizable redox abilities for catalysts [115]. The pressure gradient densities are facilitating surface reactions as a result of the reliance of electrostatic repulsion and transfer inside light-harvesting semi-conductors on crystal orientations. Furthermore, if a semiconductor is surrounded by several facets, the various electronic band topologies of the surface facets may cause spatial electrostatic repulsion, which builds up photogenerated holes and electrons for reduction and oxidation events, respectively, on distinct facets. Multi-component systems are substantially more complex than bare semiconductors because of the additional interconnections between the components.

(b) Interfacial charge: Interfacial charge transfer may be impacted by the constituent facets that combine to form the interface through solid-solid interaction in a variety of ways. As an illustration, interfacial charge transfer occurs when charge transporters are moved from the aggregate to the interface; as a result, the previously mentioned aspect-dependent energy buildup would have an impact on the charge transfer. The interfacial orientation of the energy bands, which are closely related to the constituent facets, concludes the potential alteration for causing interfacial charge transfer [116]. The charge transfer efficiency across the interface is greatly influenced by the electronic coupling and defect density at the interface, which depend on the compatibility of facet topologies (Fig. 21). As can be seen from the preceding comments, extremely effective photocatalytic materials can be produced by modifying the exposed facet on the surface and the contact facets at the interface [117]. The efficacy of photocatalytic materials is controlled by surfaces and interfaces, which are two essential factors. In addition to outline the foundations of each design, this focus review highlights

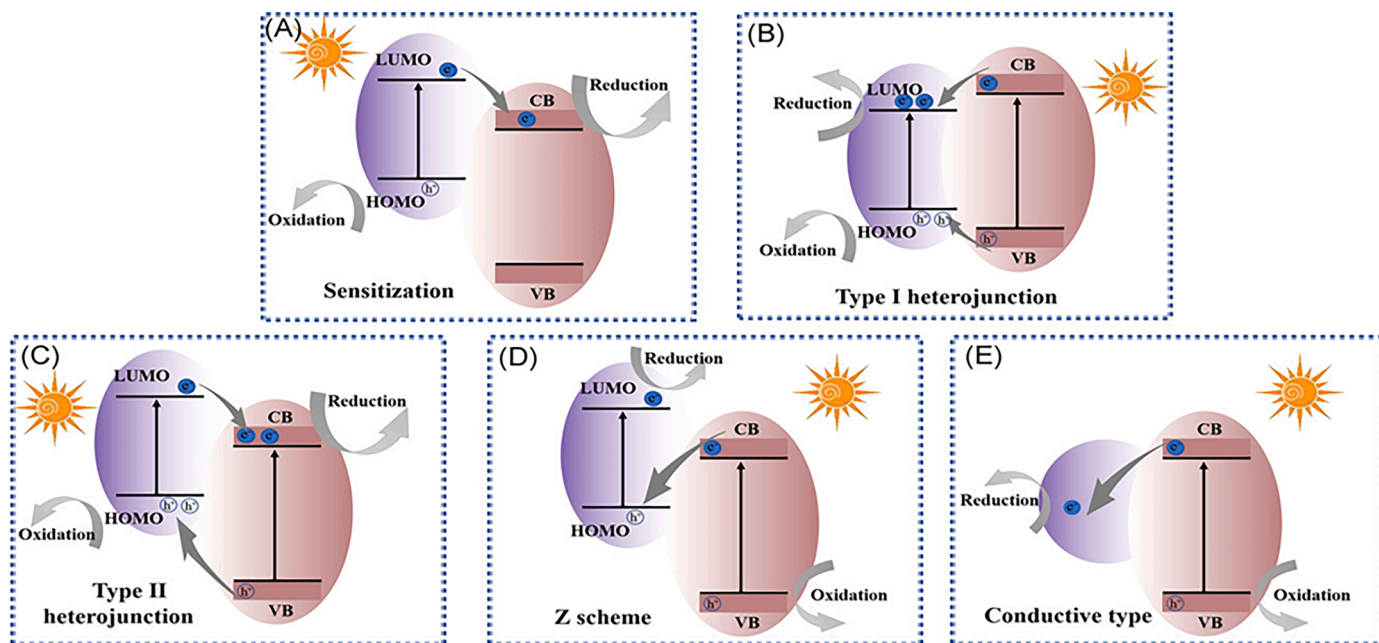


Fig. 20. A diagrammatic representation Four different charge-transfer mechanisms are shown schematically in surface hybrid photocatalysts: Heterojunction mechanisms include sensitization mechanisms (A), type I heterojunction mechanisms (B), type II heterojunction mechanisms (C), Z-scheme heterojunction mechanisms (D), and conductive types (E). Organic semiconductors are denoted by the colour purple, while inorganic semiconductors are denoted by the colour red. Acronyms for the lowest unoccupied molecular orbital (LUMO), highest occupied molecular orbital (HOMO), conduction band (CB), valence band (VB), and other terms. Reprinted (adapted) with permission from Ref. [113]. Copyright (2020) Wonyong Choi et al. Carbon Energy, Wiley Online Library. Open Access under the terms of the Creative Commons CC-BY License.

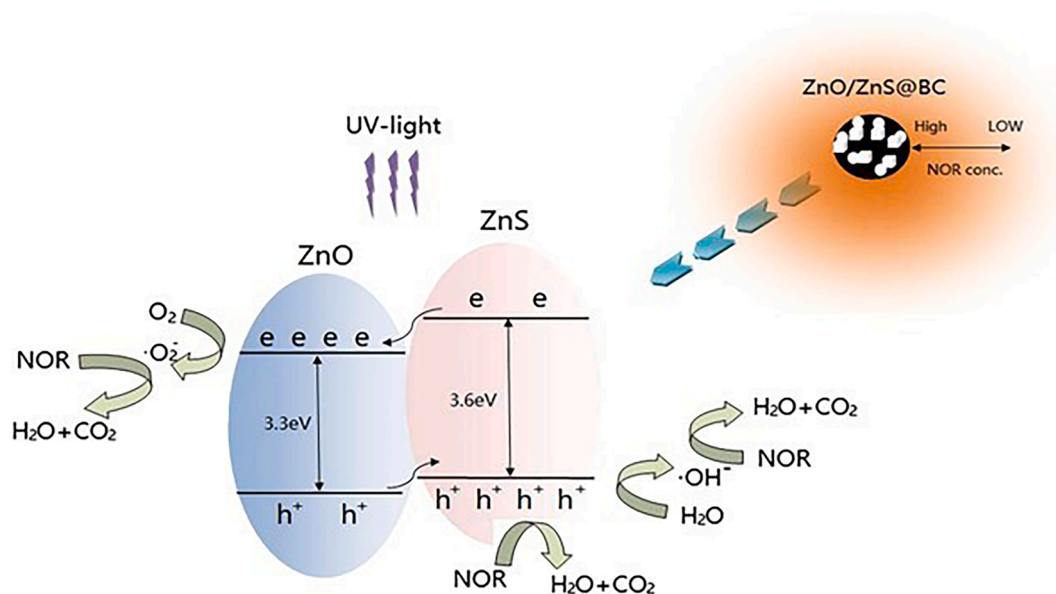


Fig. 21. Schematic representation of surface and interface reaction in photocatalysis (working principle of ZnO/ZnS@Biochar, BC). Reprinted (adapted) with permission from Ref. [118]. Copyright (2020) Yunlin Zhao et al. Scientific Reports, Springer Nature Limited. Open Access under the terms of the Creative Commons CC-BY License.

current developments in surface and interface engineering that have led to the development of extremely effective photocatalysts. The effectiveness of photocatalytic materials, especially for hybrid structures, in various reaction systems is controlled by two important factors: surfaces and interfaces.

The authors of this review describe recent developments in surface and interface engineering that have led to the development of extremely effective photocatalysts and the underlying theoretical underpinnings of those expansions [119]. The descriptions of surface and interface in the fundamental designed forms of photocatalysis are presented after an initial discussion of the functions of surfaces and interfaces in various models of charge kinetics, a crucial step in calculating the quantum efficiency of photocatalysis [120]. The authors then go on to discuss the principles of design and important standards for surface and interfaces engineering, respectively. Additionally demonstrated as an interaction effect are the connections among surface and interface elements in the creation of photocatalysts. The artificial means of manipulating the surface and interaction are summarized. Existed challenges in surface and interface technology in photocatalysis research have discussed [121]. Facet alteration of the surface and interface of photocatalytic materials has performed using a variety of synthetic ways based on the necessary understanding. Further, anisotropic etching kinetics, thermodynamic control, and facet-selective capping agents have all used to customize the exposed facets on a surface. For interface structures, however, facet engineering is more challenging.

(c) Facet engineering: Facet-dependent photodeposition, facet-dependent selective adsorption, and facet-selective capping agents have all had some degree of success up to this point [122]. Future work on interface engineering is projected to put more focus on it. By raising the proportion of surface facets with high catalytic activity or by adjusting the ratio of various facets in synergistic effects, the photocatalytic efficiency for mono-component semiconductor devices has greatly increased, and ended possibly using well-established techniques for surface engineering [123]. By logically exposing the constituent facet with the highest catalytic activity on the surface, increased photocatalytic performance for multi-component hybrid electronics has mostly been achieved using the same approach as bare semiconductors. The effectiveness of interfacial charge transfer, another crucial component for hybrid structures has been improved to some extent by choosing the right facets for interface formation, although further work is still

needed in this concern [124]. An intriguing and significant development path toward improved photocatalytic performance is the design of photocatalytic materials' surfaces and interfaces using facet engineering. In order to regulate the exposed facets of the catalytic components and enhance surface catalytic reactions, the facet-engineered surface designs for mono- and multi-component photocatalytic devices have also been developed. The dependence of surface reaction activity on exposed facets can be attributed to three main processes: (a) adsorption and reaction initiation on surface facets; (b) the surface electronic properties assemblies of different facets trying to control the redox abilities of photo-generated electrons; and (c) the accumulation of photoinduced electrons or holes on different facets.

The interface between light-harvesting and catalytic elements has indeed been designed with facets in multi-component hybrid architectures to facilitate interfacial charge transfer [125]. The three main factors that contact facets affect are: (a) the accumulation of photoinduced electrons or holes in the facets that make up the interface; (b) the interfacial band structure alignment according to the surface state structures of different facets; and (c) the interfacial electrical and structural couplings based on the facet contacts. The design of photocatalytic materials with facet-engineered surfaces and interfaces has led some potential strides recently, but it is still very difficult to fully utilize facet engineering's benefits for photocatalysis. Controlling the material interface within a multiple-component hybrid structure is, in our opinion, the most difficult assignment. The difficulty in solving this problem stems not only from the restricted synthetic methods available for manipulating the interfacial facets but also from the fact that advanced characterization approaches are needed to examine the charge dynamics at the interface (Fig. 22). Because of the serious lattice mismatch between the constituents, the synthesis of many interface structures suffers, which lowers the structural and electrical couplings at the interface [126]. Non-epitaxial growth should be an effective method for reducing the interfacial strain brought on by lattice mismatch. Having capping agents on constituent surfaces will unavoidably lower the feature of interface assemblies. For better understanding in the facets-dependent photocatalytic activities and probe the interfacial charge kinetics, high longitudinal, spectral, and sequential resolution characterization approaches are extremely desirable. To improve our comprehension of how facets, affect photocatalysis and to give facet engineers guidance in the creation of photocatalytic materials,

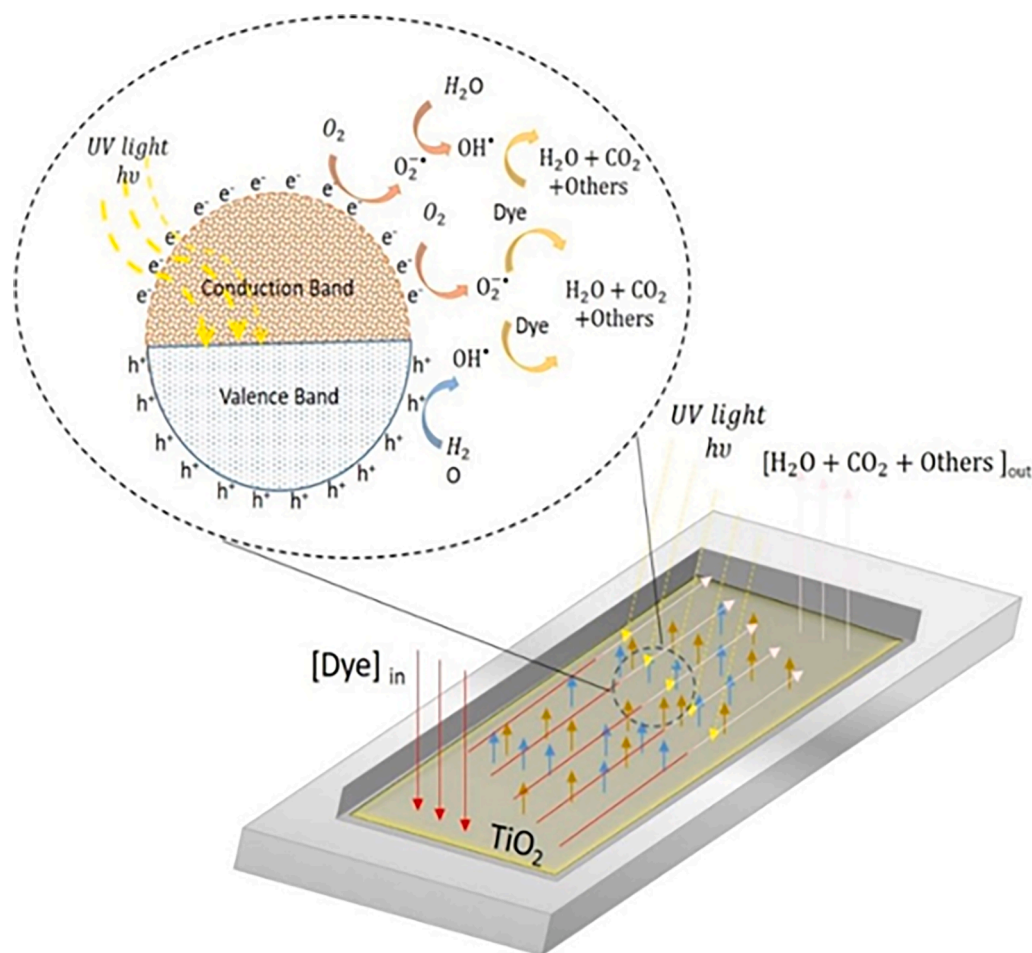


Fig. 22. Schematic representation of photocatalysis. Reprinted (adapted) with permission from Ref. [127]. Copyright (2020) Zainab Mohammed Redha et al. Arab Journal of Basic and Applied Sciences, Informa UK Limited. Open Access under the terms of the Creative Commons CC-BY License.

contemporary theoretical simulations experimental calculations are also required.

The link between facet architecture and photocatalytic performance can be shown by research in the fields of precise synthesis, complex characterisation, and theoretical simulations. This will assist build perfectly designed surface and interfacial facets for extremely proficient photocatalysts [128]. From the study above, designing the facets at a hybrid structure's surface and interface would be extremely difficult. Not only does it necessitate highly precise sophisticated synthetic processes (at the atomic level, for instance), but it also necessitates a high level of rationality due to the inherent correlation of surface with interface and the connection between structural qualities and performance [129]. Mechanistic knowledge at the interfaces of various components, such as the light absorber, co-catalyst, and passivation layers, will be crucial, similar to the previously indicated understanding of the surface of the photocatalysts. Sophisticated, integrated systems are most likely used to meet the demanding requirements for photocatalytic activity [130]. Increasingly crucial will be how these many elements interact. For instance, it is unclear whether the energy's transport through heat or light affects how a catalyst works.

Compared to similar influences at the surfaces, the influence of the many other parameters on the photocatalytic performance is understudied, except from the energetics at the interface of diverse material components. For most systems, instance, it is difficult to comprehend the specifics of the molecular level interfaces. Order to improve the interfaces even further, it is necessary to map out the electronic states that are brought about by chemical impurities and lattice mismatches in greater detail [131]. Another crucial situation to think about is how

dynamic changes to the components, which frequently occur for co-catalysts during chemical reactions, might alter the interface. It takes cues from natural photosynthesis and claims to provide a direct path to the pollution removal activity, selectivity, effectiveness, and consistency. Its progress is now being hampered by a number of difficulties, most of which are material-related [132]. Because optoelectronics and catalysis are two different, far-off domains, these problems are complicated and challenging [130]. Even nevertheless, the difficulties offer a rich environment for research, allowing for the testing of many theories and material design concepts (Fig. 23). With an emphasis on inorganic photocatalysts, the information offered in this review is merely an extensive outline of the large field. It's important to emphasize, however, that the fundamental ideas presented here are general in the sense that they can serve as fantastic sources of inspiration for the study and advancement of several catalytic reactions in which light serves as a crucial energy input.

1.8. Application of photocatalysis

Multiple energy shortages and environmental pollution issues have emerged with the evolution of society. One of the best ways to deal with issues like environmental pollution and energy depletion is through the use of photocatalysis, a new green technology that uses sunlight. There has been research done on photocatalytic technology up to this point, but additional investigation is required to enhance photocatalytic features [133]. It has been proven that vacancies play a crucial part in enhancing photocatalytic performance. In photocatalysts, oxygen vacancies have primarily been explored as a defect so far. Most of them use

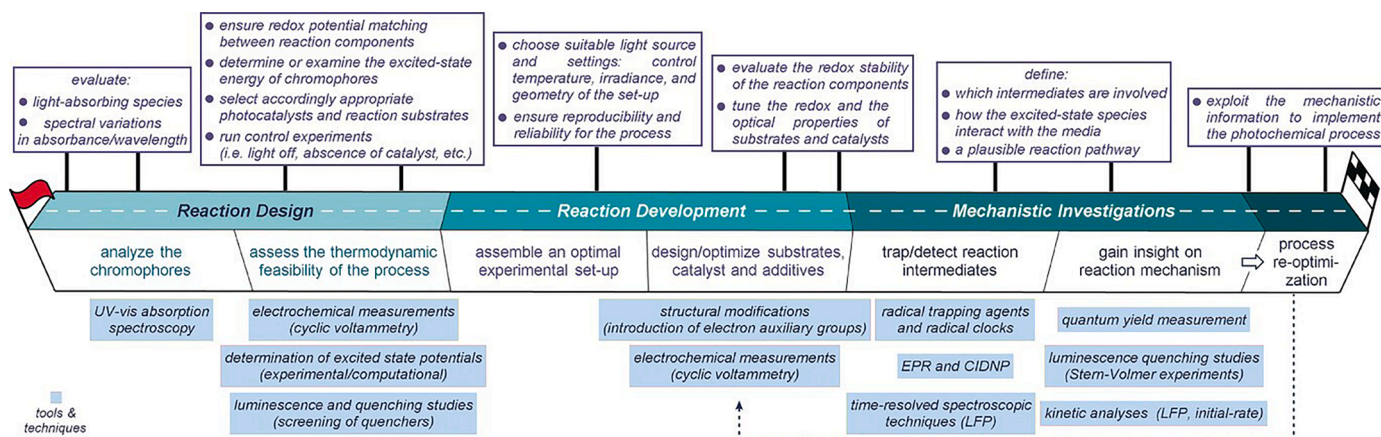


Fig. 23. A schematic illustration various application of photocatalysis. Reprinted (adapted) with permission from Ref. [48]. Copyright (2018) Paolo Melchiorre et al. Angewandte Chemie, John Wiley & Sons, Inc. Open Access under the terms of the Creative Commons CC-BY License.

oxygen vacancies to improve photocatalytic activity. Compared to other anionic vacancies, including oxygen vacancies, sulphur vacancies actually occur more readily. In this context, investigating the function and impact of sulphur vacancies on enhancing the photocatalytic activity of metal sulphides is more realistic in terms of addressing environmental issues and energy crisis. For use in the oxidation phase of wastewater treatment, photocatalysis shows considerable potential as an effective and environmentally friendly method. Photocatalysis is now at the forefront of environmentally friendly wastewater treatment and thus thanks to quick advancements in the development of innovative materials. Recent developments in photocatalytic are reviewed (Table 1). The methods for enhancing performance and how to stop degradation are the key topics of discussion. Existed difficulties and future prospects in this regards are also presented on this promising subject (Fig. 24). In order to purify water, researchers will hopefully use the informations covered in this reviewed review to innovate low-cost, high-efficiency photocatalysts [134].

The following are some significant applications of photocatalysis, including (1) discussed photocatalysts displayed potential antimicrobial properties (antibacterial and antiviral agents), (2) application of photocatalysts for rating transparent surfaces that can do self-cleaning driven by visible light, (3) using biocompatible photocatalysts *in vitro* and *in vivo* for photocatalytic cancer therapy, (4) can perform detoxification of water using cutting-edge photocatalysts, (5) applied in environmental uses for photocatalysis, such as biological pollution, air and water purifying, water disinfection, hazardous materials remediation, self-cleaning buildings, intended form, anti-bacterial action, anti-fogging resolution bleaching, [135,136]. (6) reduce the toxicity of actual wastewaters, (7) the applications relate to the treatment of air and water, green chemistry, active surfaces, and energy conversion, and they are based on the photoreduction, photoinduced, photosterilization, and photooxidation superhydrophilicity phenomena, or a combination of them, (8) applied in the food, chemical, textile, automotive, and food industries, as well as in the building and architectural, (9) used in chemical, hygiene and sanitation sectors, (10) Successfully applied in elimination of "non-biodegradable" contaminants from polluted water, (11) photocatalyst for the breakdown of organic contaminants in water based on metal oxides, (12) applied during the photocatalytic oxidation of nano metal oxides to degrade synthetic colors, [137]. (13) used as semiconductor nanomaterials made of cadmium sulphide and zinc sulphide for photocatalytic for elimination of water pollutants, (14) apply in biomass reformation by photocatalytic means, (15) applied in antiviral coatings and surfaces, (16) used to create photocatalysts based TiO₂ materials that have outstanding antibacterial and antiviral properties, (17) used in developing TiO₂ to stop against SARS-CoV-2 infection, (18) TiO₂ photocatalyst nanoparticles were produced for coating

surfaces of items and standard areas with nanoparticles based on TiO₂ photocatalysts, (19) TiO₂ photocatalyst nanocoatings may be able to halt the transmission of SARS-CoV-2 and other viruses, and (20) utilizations for photocatalysts made of graphene. Moreover, these are the following applications of photocatalytic in various processes: (a) water splitting and hydrogen production; (b) pollutant degradation; (c) organic transformations; (d) photocatalytic NO_x removal; (e) photocatalytic heavy metal ion removal; (f) synergistic photo/electrocatalysis; (g) photochemical energy conversion and artificial molecular machines (h) and solar energy conversion and photosystem II; and (i) microbial photocatalytic disinfection. A few of them were explained for a deeper understanding below diagrammatically.

(I) Synergistic photo/electrocatalysis for energy conversion and storage

In order to enhance energy conversion and storage in metal-air batteries, photo/electrocatalysis is a promising method that combines the best elements of photocatalysis and electrocatalysis [138]. This section evaluations the most current research on photo/electrocatalytic coupling reactions, notably for oxygen evolution and oxygen reduction reactions, in order to provide insight on the design principles and enhancement methods for catalysts utilized as cathodes [139].

Pretty energetic picture graph/electrocatalysts may be created to overcome battery bottlenecks in sluggish response kinetics and developed large-voltage hysteresis via know-how synergistic results and practical structure design (Fig. 25) [139]. The study found that picture graph assistance with electrochemistry can also result in more potent photoenergy consumption, which could enhance the cathode response kinetics in metal-air batteries.

(II) Photochemical energy conversion and artificial molecular machines

Utilizing sunlight as a distributed, clean, renewable energy source is essential to meeting contemporary society's energy needs in an economical and sustainable way. Over the last several decades, scientists have developed the ability to create artificial chemical systems known as molecular machines [140]. These systems use energy inputs to drive the precise motions of molecular components, which may be employed to carry out a variety of tasks [141]. Photochemical processes have been used within suitably designed (supra) molecular assemblies to create a range of light-operated artificial molecular machines [142]. These innovations may potentially open the door to the development of nano-structured materials and technologies that store, convert, and absorb light energy [143]. With the help of establishing new links with physics, biology, materials science, and floor science, the field of synthetic molecular machines and automobiles has fully matured, bringing tremendous innovation to chemistry and expanding its disciplinary man or woman [144]. Nonetheless, using artificial molecular machines for

Table 1

Latest development on photo-to-chemical energy transformation, surface and interface engineering.

S. No.	Theory	Materials and Concept	Advantage/Remarks	Refs.
1.	Electric-/magnetic-field-assisted photocatalysis	Explains the mechanisms behind static electric and magnetic fields, as well as three fundamental photocatalytic steps: light absorption, charge carrier separation, and surface reactions.	Utilizing External Fields in Photocatalysis and Energy Technologies.	[65]
2.	Converting light energy to chemical energy, and photodechlorination reaction.	Explores the utilization of cubic Cu ₂ O/Pd composite structures as photocatalytic materials for tandem catalysis.	Photocatalytic Processes: • Transforms light-based energy into chemical energy. • Highlights photocatalytic active sites and mechanisms.	[159]
3.	Photo-assisted electrocatalysts for energy conversion	Photo-assisted electrocatalysis, including photothermally aided, photogenerated carrier assisted, and LSPR-assisted enhancement, significantly impacts the carbon dioxide reduction process, hydrogen evolution reaction, and oxygen reduction/evolution reaction.	Photo-Assisted Electrocatalysis Reactions: • Charge transfer. • Surface electronic structures. • Reaction selectivity.	[160]
4.	Photosynthetic H ₂ generation and organic transformations with CdSe@CdS-Pt nanorods	Hydrogen with photon to hydrogen quantum efficiencies of up to 70 % using hybrid nanorod photocatalysts (CdSe@CdS-Pt). In addition, it utilizes solar chemical potential for oxidative chemistries, exhibiting up to 4.2 % product selectivity, photo-chemical and colloidal stability.	"Oxidative Pathways Revolutionizing Water-Splitting" • Redefining hydrogen and high-value chemicals production. • Solar refinery systems limited to efficient half-reactions or slow red-ox transformations.	[161]
5.	Chemical kinetics in solar to chemical energy and photoelectrochemical oxygen transfer reaction	Fundamental chemical kinetics formalism in photocatalysis and photoelectrochemistry, basic kinetics models for light-induced redox processes, and experimental advances in wastewater treatment using electricity or H ₂ production.	Photoelectrochemical Processes: • Measuring reaction rates for physicochemical parameters comparison. • Essential for understanding chemical interactions.	[83]
6.	Enrolling reactive oxygen species in photon-to-chemical energy conversion	Oxygen (O ₂) is an ideal chemical reagent due to its high abundance and minimal environmental toxicity. Photochemical and photophysical methods can change O ₂ 's electronic configuration, enabling more reactive forms. Role of photon-to-chemical energy conversion in reactive oxygen species (ROS), such as superoxide (O ₂ ^{•−}) and singlet oxygen (¹ O ₂), and the theory behind ROS explained.	ROS Production in Photon-to-Chemical Energy Technologies: • Overview of O ₂ — and ¹ O ₂ production. • Low activity of ambient oxygen (³ O ₂). • Aerobic oxidative reactions lead to ROS.	[162]
7.	Synergistic photo/ electrocatalysis	High-performance catalysts to address sluggish reaction kinetics and induced large-voltage hysteresis in metal-air batteries.	Photo/Electrocatalytic Coupling Reactions in Energy Conversion: • Focus on oxygen evolution and reduction. • Understand catalyst design principles and enhancement mechanisms.	[139]
8.	Photo-electrochemical conversion	Higher current densities require significant voltage input, resulting in lower solar-to-CO conversion efficiencies. Concentrated photovoltaic cell integrated into heat-managed photo-electrochemical device transfers heat to zero-gap electrolyzer cell.	Demonstration: Photo-electrochemical CO ₂ Reduction: • Facilitates resource-efficient solar fuel production. • Uses concentrated light.	[163]
9.	Solar energy conversion by photosystem II	Photosystem II (PSII) is a fascinating process that sustains life on Earth and serves as a blueprint for scalable synthetic catalysts for renewable energy applications.	Understanding PSII: • Principles of light energy conversion to chemical energy. • Molecular structures enabling these reactions.	[153]
10.	Photochemical energy conversion with artificial molecular machines	Molecular machines, synthetic chemical systems that use energy to control the movement of molecular components for specific tasks.	Artificial Molecular Machines and Light Energy: • Photochemical processes power molecular machines. • Potential for nanostructured devices. • Capable of harnessing, converting, and storing light energy.	[147]
11.	Semi-biological approaches to solar-to-chemical conversion	In-depth analysis of the advancements in semi-artificial photosynthesis, a hybrid approach to solar-to-chemical conversion that offers new ideas for a sustainable future powered by solar energy, introducing both natural and artificial photosynthesis and discussing its motivation and rationale.	Enzymes in Synthetic Materials: • Light-driven water oxidation. • H ₂ evolution. • CO ₂ reduction. • Chemical synthesis. • Incorporating microorganisms in photocatalytic and electrochemical systems.	[164]
12.	Photo(Electro) chemical energy conversion and storage	Explores the structure-property-photocatalysis relationship of graphitic carbon nitride materials, highlighting areas of agreement and unresolved areas. Molecular constituents and stacking as a quasi-two-dimensional structure, highlighting the state-of-the-art understanding.	Structural Understanding of Materials: • Examines molecular structure and impact on chemical, opto-electronic, carrier dynamics, and catalytic reactivity. • Highlights synthesis of heptazine-based materials for improved photocatalytic reactivity and light-induced electron stabilization.	[165]
13.	Directional, chiral Photoswitches with very high quantum yields	Photochromic system, diindane diazocines, has been developed to convert visible light with an 18 % efficiency to chemical energy, offering practical applications in engineering functions such as light energy conversion, molecular motors, pumps, actuators, and sensors.	High Quantum Yields in Rhodopsin: • Cis-trans isomerization yields over 70 %. • Back-reaction yields 90 %. • Two diastereomers obtained in two steps. • High conversion rates and no fatigue observed after thousands of switching cycles.	[166]

(continued on next page)

Table 1 (continued)

S. No.	Theory	Materials and Concept	Advantage/Remarks	Refs.
14.	High-performance artificial leaf: from electrocatalyst design to solar-to-chemical conversion	Sustainable energy sources are crucial for humanity's progress, especially in the face of growing population and energy demands. Converting solar energy into chemical feedstocks offers long-term storage and fuel synthesis.	Photosynthesis Overview: • Mimics direct photocatalysis, photoelectrocatalysis, and photovoltaic. • Light absorbers provide electrons for electrocatalytic reduction. • Uses holes for oxygen evolution reactions.	[167]
15.	Photo-electrochemical solar-to-fuel energy conversion by hematite-based photo-anodes – the role of 1d nanostructuring	Photo-electrochemical water splitting (PEC) is a promising method for renewable fuel production. Hematite, a metal oxide semiconductor, is a popular photo-anode material due to its high photocorrosion resistance, environmental friendliness, abundance, and low production costs.	¹ D Nanostructuring Enhances Photoelectrode Performance: • Increases surface area. • Improves directional charge transport properties. • Shortens diffusion distances. • Enhances charge lifetime and efficiency. • Compensates for hematite's weaknesses.	[168]
16.	A solar-to-chemical conversion efficiency up to 0.26 % achieved in ambient conditions	Artificial photosynthesis converts solar energy into chemical energy, offering an environmentally friendly alternative to photocatalytic methods like water splitting and nitrogen fixation.	Conjugated Polymeric Photocatalyst: Mimics NADP-Mediated Green Plant Photosynthetic Processes: • Achieves two-fold higher solar-to-biomass conversion efficiency.	[169]
17.	Energy transformations and conservation of matter and energy			
18.	Artificial photosynthesis: a pathway to solar fuels	The Intergovernmental Panel on Climate Change proposes a two-part strategy to combat climate change: transitioning to renewable energy sources and reducing fossil fuel reliance through electrification of large sectors.	Carbon Capture in Long-Haul Aviation: • Crucial for combating greenhouse gas emissions. • Large sectors struggle with decarbonization. • Need for circular carbon economy balancing fuel use and carbon capture.	[170]
19.	Furfural influences hydrogen evolution and energy conversion in photo-fermentation by rhodobacter capsulatus	The study investigates the impact of furfural on Rhodobacter capsulatus' photo fermentation hydrogen production using glucose as a substrate. The maximum hydrogen yield was obtained without furfural, but 5 mM furfural increased cell concentration by 40 %.	High Furfural Concentrations: Overproduction: • Accumulates inhibitive end-products • Underuse of substrate energy.	[171]
20.	Chemical energy sources transformations by remote experiment	Experiment uses the ISES system for control and data acquisition, with its control program and website built using the environment.	Easy Remote ISES Experiment Overview: • Understanding energy transformations in photovoltaic, electrolyser, fuel cells. • Identifying optimal regimes for maximum efficiency. • Providing perspective for experiment improvement and exploitation.	[172]
21.	Chemical approaches to artificial photosynthesis	Theory Overview: • Muckerman et al.: Calculation of thermodynamic hydricities and CO₂ reduction hydride donor design. • Horvath et al.: Electrocatalytic H₂ oxidation and production proton-coupled electron transfer mechanisms. • Lin et al.: Catalytic mechanism study for single-site water oxidation process.	Exploring Photocatalytic Processes in Solar Water Splitting: • Farnum et al. explore visible light generation of I–I bonds via Ru-tris(dimine) excited states. • Pool et al. use acidic ionic liquid/water solution for electrocatalytic H₂ evolution. • Barroso et al. study photogenerated holes in surface modified α-Fe₂O₃ photoanodes. • Smieja et al. study kinetic and structural studies in artificial CO photosynthesis. • Vagnini et al. study ultrafast photodriven intramolecular electron transfer.	[173]
22.	Recent advances on visible-light-driven CO ₂ reduction: Strategies for boosting solar energy transformation	Exploring photocatalytic CO ₂ reduction for cost-effective clean energy, but its efficiency is low due to limited light absorption, undesired charge recombination, and high CO ₂ activation barrier.	"Advanced Strategies for CO ₂ Photo-Reduction" • Tuning photocatalyst bandgaps. • Constructing heterojunctions for charge separation. • Introduction of surface defects and functional groups. • Discussing promising research for CO₂ conversion into fuels. • Recommendations for further research.	[174]

specific tasks remains a challenging goal and provides strong incentive for further research endeavors.

Molecular machines are fueled by an energy source, and their management of energy is an obvious and most desirable function [145]. Biomolecular machines beautifully accomplish this goal at both molecular (e.g., ATP synthase) and macroscopic (e.g., muscle myosin) scales. Artificial molecular machines are not limited to the blueprint established by nature but are not limited to the blueprint established by nature (Fig. 26) [146]. A critical point in this regard is the designed and effective integration of molecular devices with their environment, in order for the input energy, part of which is used to produce directed

motion at the molecular scale, to result in an effect on the surroundings which ultimately causes a sizable free energy change of the system or material.

(III) Solar energy conversion and photosystem II

Photosystem II (PSII) is a fascinating process that sustains life on Earth and serves as a blueprint for scalable synthetic catalysts for renewable energy applications. Over the past two decades, the biophysical, computational, and structural description of this process has made significant progress. The dark-stable state, semi-stable reaction intermediates, and transient states of PSII have all been shown to have high-resolution crystal structures [148]. The fundamental ideas behind

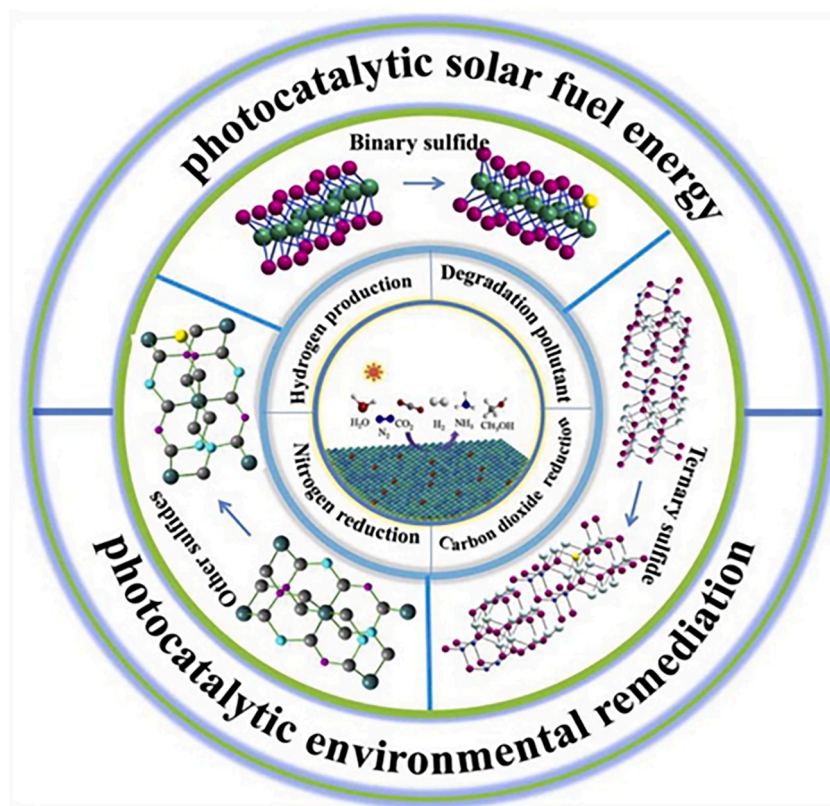


Fig. 24. An illustration of application of photocatalysis. Reprinted (adapted) with permission from Ref. [130] Copyright (2022) Wei Zhou et al. Chem Catalysis, Elsevier. Open Access under the terms of the Creative Commons CC-BY License.

the transformation of light energy into chemical energy and the molecular structures necessary for these reactions are the main areas of current PSII understanding [149]. Each monomer of the cyanobacterial PSII core has 17 integral membrane proteins, 3 peripheral proteins, and over 80 cofactors. The crystal structure shows the presence of over 1300 water molecules per PSII monomer, mostly located in regions close to the cytoplasm and in the luminal extensions of PSII [150]. Three water filled channels have been identified on the luminal side that connect the lumen with the site of water oxidation, the Mn_4CaO_5 cluster, regulating water access and facilitating the egress of protons [151,152]. Additionally, channels at the plastoquinone site (QB site) for proton transfer from the outer water phase and for the entry of PQ and the 'ejection' of PQH2 are also present.

(IV) Photocatalytic nanomaterials for blocking the SARS-COV-2 spread

Due of the ongoing global epidemic caused by COVID-19, best methods to stop the transmission of germs are now more well known. In this regard, there has been a resurgence of interest in the research into developing a surface that either eliminates or prevents the adhesion of microbial organisms [153]. There are several study reports available on the application of antibacterial materials or coatings, but the amount of information on the usage of antiviral materials is far less [154]. But as more research is done in this area, the literature is continually updated. Combining antibacterial and antiviral chemical agents is a potentially revolutionary method to inhibit the spread of disease-causing germs [155]. In this review, a wide range of antibacterial and antiviral substances, were examined including those generated from copper, silver, biodegradable polymers, small-molecule organics, artificial and TiO_2 (Fig. 27) [156]. In-depth discussion of the surface defence mechanisms used by the materials against pathogen colonies brings out the essential distinctions that might set the parameters for the future creation of enhanced antibacterial and antiviral substances and surfaces [157].

With the present coronavirus pandemic affecting the entire world, it

is important that new materials, medicinal advancements, or technological advancements be made in order to combat the SARS-CoV-2 infection. Although the exact mode of SARS-CoV-2 transmission is not being properly investigated, it appears to spread through water, air, and surfaces. Consequently, it is necessary to continuously sanitize the area in which you live. It is important to look into products for this purpose that are highly powerful against viruses, affordable, eco-friendly, and practically usable. Under ultraviolet light, titanium dioxide (TiO_2) has a potent oxidative action and is used in the biomedical area as a photocatalytic disinfectant. TiO_2 based photocatalysts have the potential to be employed even in interior environments to inactivate bacteria and viruses because they are powerful antibacterial and antiviral agents in ambient circumstances. It's interesting to note that current research proved TiO_2 photocatalysts to be successful in eradicating SARS-CoV-2 [158]. The potential of TiO_2 photocatalysts as an emergent antimicrobial against SARS-CoV-2 infection has indeed been reviewed, given their good antibacterial and antiviral activities against a variety of microorganisms and viruses. The current stage of the development of TiO_2 based nano-photocatalyst as a disinfectant demonstrates their capacity to combat SARS-CoV-2 viral infection and is promising for any other such modifications or viruses, microorganisms in future trials.

2. Conclusion

The discovery of the rate-determining processes in photocatalysis is advantageous for the design and production of highly effective and discerning photocatalysts. With a focus on the following domains; photoelectrocatalytic reactions, band-gap engineering of photocatalysts, surface science of photocatalysis, mathematical modeling, probability and evaluation of the photocatalytic degradation, Monte Carlo simulation, analogy analysis of electro catalytic water splitting, reconsidering the description of photocatalysis, energy bands and energy levels, by considering emerging scientific opportunities in surface

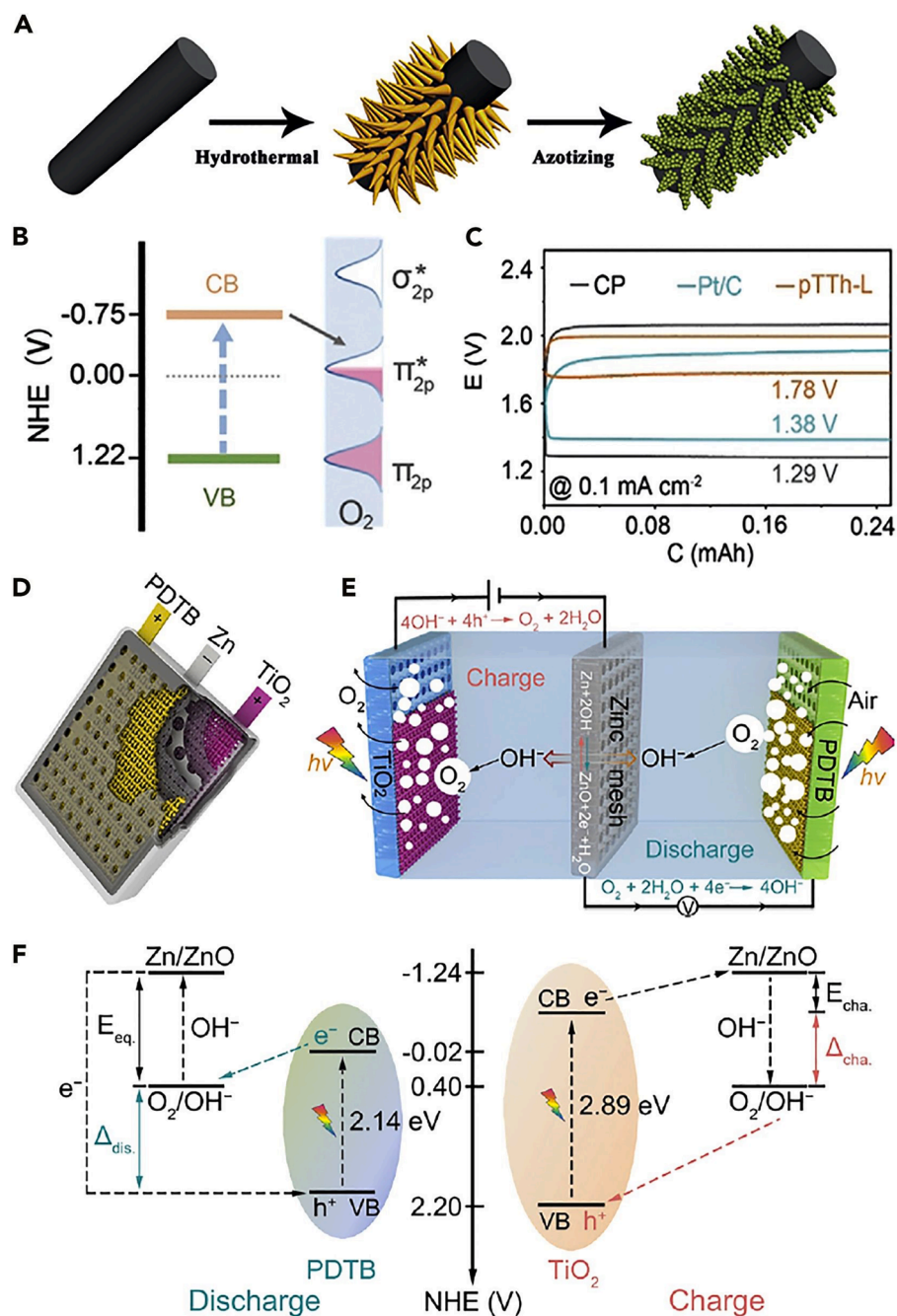


Fig. 25. An illustration of photo/electrocatalysis for metal-air batteries. Reprinted (adapted) with permission from Ref. [139]. Copyright (2021) Yu Zhang et al. Matter, Cell Press. Open Access under the terms of the Creative Commons CC-BY License.

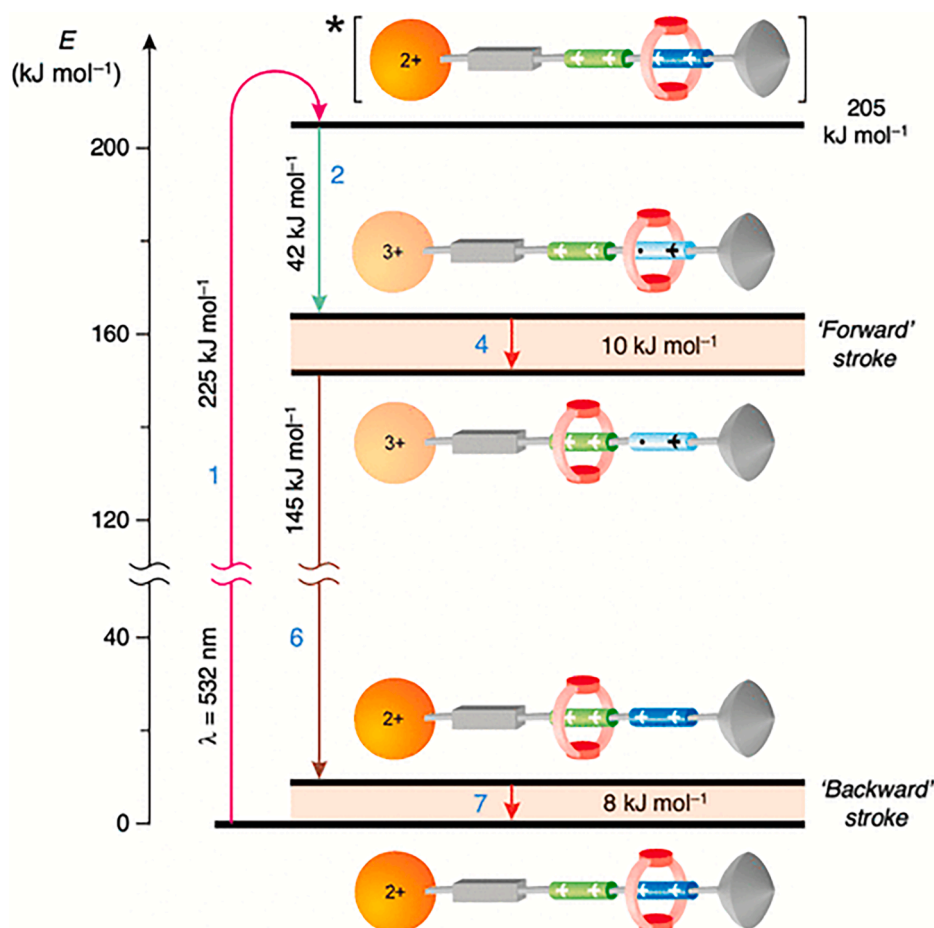


Fig. 26. A diagram of energy-level diagram showing how rotaxane 2 operates as a self-sufficient, reversible chemical shuttle powered by visible light. Reprinted (adapted) with permission from Ref. [147]. Copyright (2021) Alberto Credi et al. Energy Fuels, American Chemical Society. Open Access under the terms of the Creative Commons CC-BY License.

engineering and interface modification for shaping of photocatalysis, the application of photocatalysis, and photocatalytic nanomaterials for blocking the SARS-CoV-2 spread, the authors elaborate the current state of knowledge, and cutting edge aspects of critical research in the field of photocatalysis. Different aspects of photo-to-chemical energy transformation achieved by pioneering photocatalysts, and surface and interface engineering in particulars was explored further. The future directions of fundamental and applied photocatalysis and thermal catalysis are also described. Moreover, the catalysis initiated by solar radiation, including (i) investigations into structured molecular assemblies, (ii) simple molecular systems, (iii) semiconductors as photocatalysts, (iv) selective organic synthesis via photocatalysis, (v) the application of photocatalysis to combat environmental issues, (vi) current advancements and prospects of solar radiation-induced photocatalysis and thermal catalysis applications proposed for the future in the field of solar energy, and finally (vii) the anticipated role of photocatalysis in the global atmosphere's chemistry has been articulated. Moreover, surface changes at the molecular level during photocatalytic degradation have been extensively studied using theoretical and mathematical derivations. Furthermore, to gain a better understanding of the reaction interface, theoretical calculations and experimental data have merged.

Materials' physicochemical qualities of have a substantial impact on the catalytic activity toward photocatalytic degradation processes. Here, authors underlined various conditions such as catalysts with lower doses and quicker kinetics can cut developmental costs and increase the intensity of photocatalytic degradation processes. The capacity of photocatalytic degradation to be increased is projected to be greatly aided by

the following techniques: surface tethering, heteroatom doping, size control, crystal facet engineering, defect engineering, and defect engineering. Moreover, it is important to thoroughly examine the impacts of different variables, including photocatalyst concentration, solution pH, inorganic ions, temperature, and light source on the effectiveness of photocatalytic water treatment. Additionally, to prevent corrosion during photocatalyst water treatment, it is crucial to fundamentally improve semiconductors' optical stability. Besides, the efficacy of light source usage and the effectiveness of light transfer inside the reactor are crucial to the design of the reactor's efficiency and the practical use of photocatalytic technology.

An outlook on potential future lines of inquiry within this extensive field of study is given in the final section. This review is an irreplaceable resource for various disciplines because of its in-depth illustration of the topics including thorough understanding on engineering of materials, and applied devices. The authors review important findings related to surface science underlying several traditional and novel photocatalysts applied for environmental and energy applications, with a focus on key interface activities in photocatalysis, such as interfacial charge transfer, the role of co-catalysts, and adsorption over the photocatalyst surface [73]. This review serves will be assisted as a helpful reference for both beginners and experienced researchers in photo-to-chemical energy transformation, pioneering photocatalysts, surface and interface engineering by comprehensively and timely reviewing the state-of-the-art of the surface art in photocatalysis. Recently published reviews have been studies for exploring surface science and photocatalysts in a timely manner. The application of mathematical equations has provided new constraints for representing the prospect that a photon is received by the

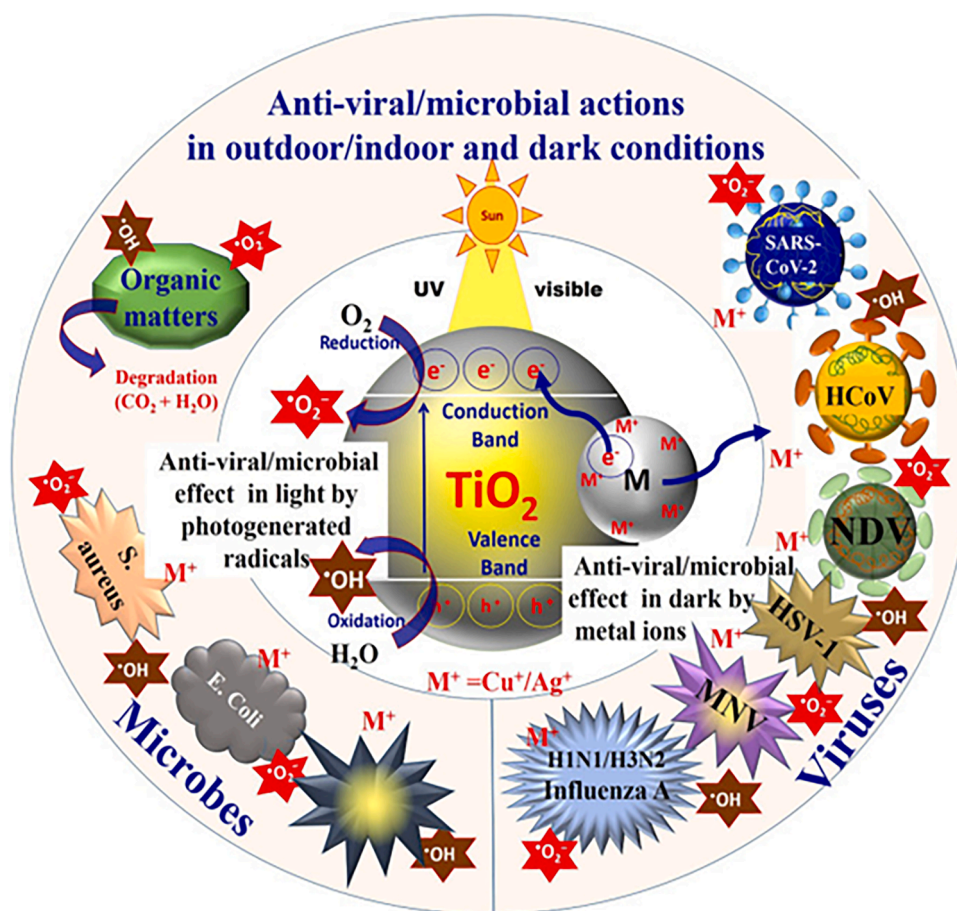


Fig. 27. An example of TiO_2 -based photocatalysts and their role in the breakdown of organic materials, as well as their antibacterial and antiviral properties against various microbes and viruses. Reprinted (adapted) with permission from Ref. [154]. Copyright (2022) Yogendra Kumar Mishra et al. Micro and Nano Engineering, Elsevier. Open Access under the terms of the Creative Commons CC-BY License.

photocatalytic suspension while forming an oxidizing radical. In the referred mathematical elucidation, it was perceived that the probability was associated with the two foregoing stages. In the end, various applications of photocatalysis and the application of photocatalytic nanomaterials for blocking the SARS-CoV-2 spread are underlined and presented in detail.

Availability of data and materials

Wherever necessary, relevant citations are included in the reference section.

CRediT authorship contribution statement

Rajiv Kumar: Writing – original draft, Resources, Investigation, Data curation. **M.P. Chaudhary:** Writing – original draft, Resources, Data curation. **Amir Al-Ahmed:** Writing – review & editing. **Somnath Bhattacharyya:** Writing – review & editing. **Svetlana von Gratowski:** Writing – review & editing, Validation. **Jibran Iqbal:** Writing – original draft, Resources. **Inamuddin:** Writing – original draft, Supervision, Methodology, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Inamuddin reports financial support, administrative support, article publishing charges, equipment, drugs, or supplies, statistical analysis,

travel, and writing assistance were provided by Aligarh Muslim University. Inamuddin reports a relationship with Aligarh Muslim University that includes: employment. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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