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Review

Photocatalytic Application of Polymers in Removing Pharmaceuticals from Water: A Comprehensive Review

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Abstract: This comprehensive review covers recent advancements in utilizing various types of polymers and their modifications as photocatalysts for the removal of pharmaceutical contaminants from water. It also considers polymers that enhance the photocatalytic properties of other materials, highlighting their dual role in improving water purification efficiency. Over the past decades, significant progress has been made in understanding the photocatalytic properties of polymers, including organic, inorganic, and composite materials, and their efficacy in degrading pharmaceuticals. Some of the most commonly used polymers, such as polyaniline, poly(p-phenylene vinylene), polyethylene oxide, and polypyrole, and their properties have been reviewed in detail. Physical modification techniques (mechanical blending and extrusion processing) and chemical modification techniques (nanocomposite formation, plasma modification techniques, surface functionalization, and cross-linking) have been discussed as appropriate for modifying polymers in order to increase their photocatalytic activity. This review examines the latest research findings, including the development of novel polymer-based photocatalysts and their application in the removal of pharmaceutical compounds, as well as optimization strategies for enhancing their performance. Additionally, challenges and future directions in this field are discussed to guide further research efforts.

Keywords: pharmacologically active compounds; drugs; water contaminants; modification of polymers; catalytic materials; sustainable water treatment; environmental protection; wastewater

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1. Introduction

The aqueous environment plays a central role in the water cycle and the world's ecology and is a major component of various forms of human activities [1]. Water pollution with residue amounts of various chemicals, including pharmaceuticals, pesticides [2], dyes, etc., creates a lot of serious environmental problems [3–5]. The main reason for the spread of pharmaceuticals is the treatment of various diseases, as well as the so-called pro-pharmaceutical effects [6]. The appearance of pharmaceutical substances in the environment also concerns the emission of veterinary-connected preparations [7,8]. The impact of various factors on the behavior and properties of pharmaceuticals in wastewater, natural bodies (rivers, lakes, seas), and technical water has significantly expanded our understanding [9].

Today, the most common technologies used for the removal of pharmaceutically active compounds include reverse osmosis, ultrafiltration, nanofiltration, activated carbon, and many others [10–12]. However, these processes do not entirely remove pharmaceuticals from the water. The inefficiency of conventional methods in wastewater treatment and the removal of pharmaceutical compounds from wastewater have become a global concern [13,14]. Advanced oxidation processes (AOPs) showed great potential and played a prominent role in the complete removal of pharmaceuticals from water sources and the environment. One of the most often used AOPs is photocatalysis [15]. In this process, photocatalytic materials, whose activation is induced by light emission, take a primary role. The application of nanotechnologies for removing pharmaceuticals from water is widely used [14]. Nano-sized photocatalysts, such as TiO_2 [16], ZnO [17], etc., are widely used. However, nowadays, new polymer materials [18] and their modifications are used very often, side by side with TiO_2 and ZnO [18,19].

Since the number of research studies regarding the efficiency of polymers has expanded in recent years, there is a need for a more comprehensive review of polymers as a promising sustainable material for photocatalytic applications in water treatment [20,21]. Therefore, the current work intends to encompass all significant studies on sustainable polymer materials for the elimination of pharmaceuticals from water and wastewater. This review is divided into several sections. Information on sources, problems, occurrences, and potential risks of pharmaceutical compounds are discussed first. The next section presents a critical examination of various polymer materials and their modifications used in photocatalytic processes from both experimental and computational approaches. Further, the efficiency of different polymer modifications in the removal of pharmaceuticals from the environment is addressed in detail. The most important advantages and challenges of using polymer materials are addressed, as well as their limitations.

1.1. The Problem of Pharmaceutical Pollutants in Water

The production and consumption of pharmaceuticals have increased dramatically in recent decades [22], leading to the emergence of water-soluble and pharmacologically active organic micropollutants [23,24]. These pollutants can be found in water sources and ecosystems as parent compounds or as metabolites [25]. Pharmaceuticals present in the environment can change the composition of the natural flora and fauna [26], as well as the structure of the entire ecosystem in the aquatic environment [27]. They are frequently found in wastewater (Table 1), surface water, and groundwater, where they have raised concerns due to their environmental impact and the ineffectiveness of conventional treatment plants in removing them [28]. The presence of pharmaceutical pollutants can lead to the pollution of ecosystems [29] and the exchange of carbon, nitrogen, and phosphorus within cyclical processes. One of the responses to this environmental challenge is the emergence of new technology and materials, in particular, the use of AOPs [30–33]. The appearance of pharmaceuticals in the environment can have severe consequences and can generate resistance to certain drugs in aquatic organisms, humans, and animals [34].

From an economic point of view, the cost of removing pharmaceuticals in water treatment plants [35], which requires the development of increasingly efficient treatment technologies, is very high, since pharmaceuticals are present as residues in these waters [36,37]. In order to satisfy current demands without affecting the environment, it is essential to provide a long-term solution for pharmaceutical removal from the environment based on social, technical, economic, and environmental conditions in a sustainable way [38–41]. Among AOPs, photocatalysis stands out [42]. One of the new materials utilized in photocatalysis is sustainable polymers [43,44]. Photocatalytic polymer-based degradation stands out as a potential approach for the removal of pharmaceuticals from the environment [45] since it typically requires little energy, has low operation costs, and, most importantly, does not produce any toxic by-products that cause secondary contamination [46]. Also, polymer materials can interact with the transformation products made in the photocatalytic degradation process. The advantages of polymer-assisted preparation procedures are mainly the speed of the synthesis and maturation around the matrix surface and improved polymer adhesion/anchorage of the anchored oxides. However, little is known about the effect of the formation of small molecules as products of photocatalytic reactions in situ on the anchored oxides or their interaction with the matrix-to-supported oxide binding. The interactions of photodegradation products with polymers can be of importance for many potential products. The products of photocatalytic degradation of pollutants are often deposited or adhered to matrix materials like polymers. This may affect their properties, determined by chemical as well as physical interaction and binding to the surface. Polymer-modified properties of those materials, as matrices for photocatalytic degradation, have recently been successfully applied for wastewater purification, self-cleaning surfaces, and surfaces with photobiocidal properties. This would allow for an extremely easy one-step preparation of photocatalytic-polymer based reactive materials, used for degradation of both parent compounds and photodegradation products, thus backing up the economy of their implementation [47–49].

Table 1. Detection of pharmaceuticals in different wastewater.

Pharmaceutical	**Location**	**Analysis Method**	**c (ng/dm^3) Detected in Effluents**	**Reference**
Amoxicillin	Kisii and Kabarnet wastewater treatment plants in Kenya	HPLC–UV/Vis	90	[50]
Ampicillin	Olomouc region, Czech Republic	UPLC–TQ-S/MS	48	[51]
Azithromycin	Sanya, China wastewater treatment plants	HPLC–UV/Vis	56,600	[52]
Carbamazepine	Czech wastewater treatment plants	UHPLC–MS/MS	730	[53]
Cephalexin	Pharco B International Pharmaceutical Company in Borg El Arab, Alexandria, Egypt	HPLC–DAD	71,900	[54]
Ceftazidime	Pharco B International Pharmaceutical Company in Borg El Arab, Alexandria, Egypt	HPLC–DAD	94,000	[54]
Ceftriaxone	Pharco B International Pharmaceutical Company in Borg El Arab, Alexandria, Egypt	HPLC–DAD	170,300	[54]
Clarithromycin	Neringa (Nida) wastewater treatment plants	HPLC–UV/Vis	15	[55]
Chloramphenicol	Kanchipuram District, Chennai	GCE	39	[56]
Ciprofloxacin	Sanya, China wastewater treatment plants	HPLC–UV/Vis	24,000	[52]
Doxycycline	Machakos, wastewater stabilization ponds	LC-ESI–MS/MS	1500	[57]
Erythromycin	South Africa, untreated wastewater	LC–MS/MS	55	[58]
Metoprolol	Czech wastewater treatment plants	UHPLC–MS/MS	960	[53]
Metronidazole	Czech wastewater treatment plants	UHPLC–MS/MS	7500	[53]
Naproxen	Czech wastewater treatment plants	UHPLC–MS/MS	980	[53]
Norfloxacin	Machakos, wastewater stabilization ponds	LC–ESI–MS/MS	2900	[57]
Oxytetracycline	Dhaka wastewater effluents in Bangladesh	RP–HPLC–UV/Vis	670	[59]
Paracetamol	Czech wastewater treatment plants	UHPLC–MS/MS	82,500	[53]
Propranolol	San Luis Province, Argentina	HPLC–DAD	850	[60]
Roxithromycin	Nicosia wastewater, Cyprus	SPE–DEX	700	[61]
Sulfadimidine	Shanghai wastewater treatment plant	UPLC–DAD	440	[62]
Sulfamethoxazole	Czech wastewater treatment plants	UHPLC–MS/MS	7500	[53]
Tetracycline	Bouc-bel-air, France wastewater	UPLC–FLD	4820	[63]
Tramadol	Czech wastewater treatment plants	UHPLC–MS/MS	3500	[53]
Trimethoprim	Czech wastewater treatment plants	UHPLC–MS/MS	3000	[53]

1.2. Objectives and Significance of the Study

Photocatalysis by semiconductors has been recognized as one of the most acceptable, sustainable, and eco-friendly techniques to mitigate increasing pollution of the environment [64]. However, commercialization of these advanced technologies is challenging due to the poor activity of pure semiconductor photoactive material, charge recombination, and light absorption only in the ultraviolet region of the solar spectrum [65,66]. Evolution in the materials science area has led to the use of various polymers as adequate support for semiconductor photocatalysts, providing solutions for the challenges mentioned above [67,68]. This might be attributed to the very low recombination of photogenerated charge carriers (electron–holes, e^{-}–h^{+}), which possess a long carrier lifetime due to the heavy adsorption of semiconductor nanocrystals onto polymer support [69]. The introduction of a polymer barrier band can increase photocatalysts' response to visible light owing to the narrow band gap, and they can also act as effective scavengers of photo-generated holes [70].

Photocatalysis is a green technology [71], and from this perspective, polymers are concurrently applied without employing supporting semiconductors for wastewater purification [72]. Polymers have several distinct advantages as photocatalysts [73] over conventional metal oxides, semiconductors, and inorganic nanocrystals, including turgid backbones, controlled porosity, excellent chemical durability, well-defined micropores, strong chelation sites for favorable interactions with transition metal centers, and flexibility in maintaining conjugation in extended structures [18,74,75]. Organic polymers could provide an alternative to toxic and bioaccumulative heavy-metal-containing semiconductors, especially in biomedical and environmental remediation applications [76]. Still, polymeric materials exhibit low absorption in the visible spectrum of sunlight [77]. This problem can be dealt with by introducing photoactive species, including conducting polymers and TiO_2 [78]. Currently, conjugated polymers are recognized for their additional application as visible-light active photocatalysts owing to their long excited-state lifetimes, high quantum yields, and outstanding photostability [79,80]. The major challenge is enhancing the photocatalytic degradation of recalcitrant organic waste in environments where stable, reliable, and benign aromatic (homo)polymers can offer structural and functional sustainability under a wide range of operational conditions [81].

In the history of the development of organic and inorganic chemistry, inorganic nanoparticles, nano capsules, and nano complexes have been used in combination with organic polymers as reaction media for many organic modifications. Their easy methods of preparation have been mediated by chemical and physical procedures [82]. Organic polymers are used as supported/reducing/dispersing/capping agents in most cases of synthesis of such inorganic nano catalysts as reaction media. Polymers are seemingly the best choice as reaction media in the presence of nano catalysts due to their ease of separation, recyclability, low cost, and non-corrosive, reusable, non-toxic nature in mediated synthesis. Polymers have been widely used as reaction media in combination with various nano catalysts in different organic transformations [83]. Organic nano catalysts, polymer nanocomposites, and support polymers have been comprehensively used in combination with molecular catalysts, nano catalysts, and metal-free catalysts. Such polymer-supported nano catalysts have offered a unique benefit in organic synthesis with the development of many magnetic, non-magnetic, and semi-magnetic complex nano hetero molecules, which have been used in many organic transformations and minimize the volume of toxic waste and disposal of products due to their reusability in the organic transformation, and offer economy and safety along with the environmental sustainability of the desired products [84]. The use of TiO_2 nanoparticles is attracting increased attention in various technological, environmental, and biomedical applications. In turn, polymers, with their broad spectrum of physical characteristics, processability, tailorable biodegradation, various related substances, responsiveness to external stimuli, and low production cost, are widely used in different areas such as medicine, biotechnologies, environmental uses, drug delivery, dentistry, cosmetics, clothing, packaging, and rarefied gas separation [85]. ZnO is an essential technological material. The popularity of ZnO is due to the fact that zinc oxide nanoparticles possess and manifest various physical properties, as well as the nature and characteristics that are a consequence of the peculiarities of nanoparticle formation and growth. Furthermore, ZnO also has broad applications relative to various sectors and could be used to realize a variety of sensors. ZnO and polymers have a number of properties, the combination of which allows for the realization of a wide range of composite material properties. According to the requirements of protective coatings, the most essential property is protection against ultraviolet and visible light. Some polymers have an enhanced absorption capacity in these particular ranges. In many areas, polymers can effectively compete with more expensive inorganic materials [86,87].

2. Polymers for Photocatalytic Applications

Rapid advancements in interdisciplinary scientific research on hybrid green functional materials, incorporating functional elements for advanced electronic, ionic, and photonic functionalities, continue to facilitate elusive clean energy production, toxic pollutant clean-ups, and safe biologically relevant reductions and hydrogenation chemistries [88,89]. The cost-effective synthesis, facile band manipulation, and straightforward nano-modularity of polymeric photocatalysts are, broadly speaking, the main reasons for increasing research and application attributes [90]. The combination of a synthetic environment and tapping malleable surfaces of photocatalysts often causes an active photocatalytic face to interact charge distribution with electro-photonic and integrated photogenerated product storage and cycles [91].

The versatility of polymers in the industry lies in the ability to combine different compounds to form polymers and mold them into any desired shape, and subsequently apply desired properties, or make chemical modifications to obtain value-added polymers. Polymers can be used in the form of powders, membranes, foams, surface loads, etc. [92–95]. Polymer powders are defined as finely divided, solid, spherical plastics that are made from combinations of bulk or solution polymerization and processing technology. These spherical particles may have diameters ranging from a few micrometers to over 200 μm. Powdered polymers are essential in terms of form, economics, aesthetics, and chemistry. For practical use, a polymer powder must have a basic elemental composition, suitable physical characteristics, and uniform properties when sampled [96]. Polymer membranes are generally synthesized from organic solvent mixtures involving polymers and additives and need to be prepared in films. According to its intended application, the polymer type/dosage, concentration, crosslinking density, film thickness, and any additives can be chosen to meet different aims, and can include materials like polysulfone, polyetherimide, cellulose acetate, poly(vinylidene fluoride), and others. Utilizing polymer membranes could be preferable owing to their exceptional properties such as structure, surface modifications/enhancements, hydrophobic/hydrophilic balance, size, function, and cost for specific applications. Despite the possibility of using them in different ways, polymer membranes have some disadvantages, such as fouling and low water flux [97]. During the current era of agricultural and environmental concerns, interest in biodegradable and renewable polymer foams is increasing. Importantly, the properties of porous foam are intimately linked with the processing technology used in foam formation. Therefore, manufacturing processes and techniques for novel polymer foams are constantly improving. Due to their unique properties and performance, polymer foams have achieved significant improvements in product performance, cost-effectiveness, weight reduction, etc. [98]. Polymers, having a wide variety of properties and chemical compositions, are currently serviceable in a number of applications, including packaging, electrical insulation, and protective coatings. Many advantageous and valuable properties of polymers are realized in the performance of surface functions. The characteristics of polymers' surfaces are often complex, qualitatively different, and sometimes unpredictable from data on their bulk state. Polymeric materials are classified into semicrystalline, amorphous, or glassy forms; usually, polymers have complex chemical, physical, and mechanical natures, and exhibit a great range of properties. Polymer surface engineering is both necessary and interesting from a variety of technological perspectives. It can involve structural organization at several length scales, ranging from the small or nanostructured surface topographies (length scale < 100 nm) of coatings and adhesive adhesion devices to macroscopic-scale patterns (length scale > 1000 μm) [99].

Due to the distinctive chemical and physical properties of polymeric materials, they are considered suitable and promising candidates for AOPs [100,101]. The advantage of using polymers as sensitizing agents in photocatalytic composites is that they may contribute to improving photocatalytic efficiency due to π-conjugated systems containing high concentrations of electron-rich species, which are available for transfer in the semiconductor's conduction band [102]. Also, it has been proved that by using polymer materials, recombination of photo-generated charge carriers is reduced, while conductive polymers tune the semiconductor's band gap [103]. Based on density functional theory models, conducting polymers such as polyaniline, poly(p-phenylene vinylene), polyethylene oxide, polypyrrole, polythiophene, poly(1-naphthylamine), polycarbazole, polyacetylene, poly(3,4-ethylenedioxythiophene), and poly(o-phenylenediamine) exhibit visible absorption activity due to their low band gap values, which makes them ideal candidates for extending the semiconductor's range of light absorption [104,105]. Also, conjugated mesoporous polymers and, subsequently, covalent triazine frameworks are widely used for visible light-induced photocatalysis [106]. These bulk systems are large-scale conjugated systems with defined nanostructures, maximizing surface area and, therefore, allowing an efficient photocatalytic process [107].

Over the past few decades, research endeavors have been intensively devoted to finding suitable photocatalysts for practical applications [108]. Among them, polymers have gained attention as promising candidates for many photocatalytic applications (Figure 1) [19]. Some of the most often used polymers in photocatalytic reactions are polyaniline, poly(p-phenylene vinylene), polyethylene oxide, polypyrrole, polythiophene, poly(1-naphthylamine), polycarbazole, polyacetylene, poly (3,4-ethylenedioxythiophene), poly(o-phenylenediamine, etc. [104,105].

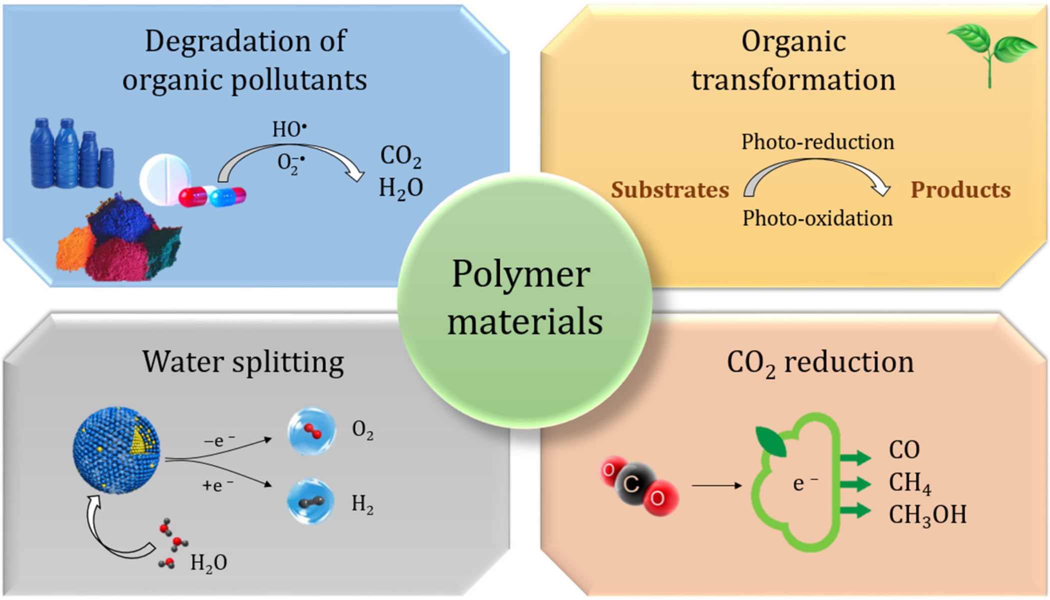

Figure 1. Overview of various photocatalytic applications of polymers. Reprinted with permission from Ref. [19], copyright Royal Society of Chemistry.

2.1. Types of Polymers Used in Photocatalysis

The fundamental classification of polymers:

i. Inorganic polymers. They represent aluminosilicate-based materials, which are conventionally produced by the activation of solid alkali silicate. Geopolymers are inorganic polymers, considered a subset of inorganic polymers since the aluminosilicate network is coordinated tetrahedrally and primarily has aluminum atoms and silicon [109]. These materials are flammable, durable, resistant to rust, and nonpoisonous. Inorganic polymers based on silicon are widely employed in water purification treatment due to their large surface area, electrical conductivity, stability, flexibility, and reusability. The inorganic polymers with silicon and phosphorous in their structures have large bond angles and bond lengths, while their bonds are more ionic [110,111]. Even at low temperatures, they retain elasticity. They can withstand very high temperatures in an oxygenated atmosphere since these polymers have more inorganic elements. Inorganic polymers are highly resistant to homolytic dissociation. As a consequence of their inorganic networks, these polymers are resistant to UV and high-energy irradiation, owing to their optical transparency throughout a narrow wavelength range and stronger inorganic connections [112]. Typically, in an inorganic polymer, the microstructural elements are built from three-dimensional arrays of oxygen, E-O-E, where E is an element such as Si, Al, P, or B, through linkage with either oxygen or other heteroatoms [113]. The mechanism that joins the silicon–oxygen–silicon links, characteristic of siloxanes, has substantially varying hydrophobic or hydrophilic stability according to the size and the polar character of the molecular affine groups, which are silicon polymeric units in a nonpolar environment, differing from the glycol groups. These polymeric membranes polymerize the silicon and oxygen cycles near the parent alkoxide, which is produced with high reactivity, and which can be used in polyester acrylate copolymeric coatings. Inorganic silicon-based polymers must undergo heat treatment for reactivity and their final application (biomaterials, photocataysis, optical devices, energy storage) [114]. Polymers containing a main-chain of boron are an interesting and important class of materials that have applications in several fields such as liquid-crystal materials, photoresist materials, nonlinear optics, boron neutron capture therapy, fire retardants, and inorganic binders. Boron-based polymers and inorganic polyboron clusters with isolable boron–boron, boron–oxygen, and boron–carbon linking atoms have long attracted widespread interest in both pi-conjugated all-boron and pi-conjugated all-boron-containing polymers to expand the palette of functional molecular and polymeric materials, including (opto) electronic, (non) linear optics, magnetic, electrical, and chiral properties. In addition to the inherent upper chalcogenide boron clusters, hexacyclic structures are valuable as a building block for the design of advanced high-level functional building blocks, with the stabilization of the resultant polymers using flexible moieties, porphyrins, and donor-acceptor [115]. While a small number of chemical elements, such as carbon and silicon, have become highly important in the development of new types of polymers, other atoms that are used much less frequently, such as phosphorus, can build polymers with unique and distinct properties. Of particular note for phosphorus-based polymers is the inherent flame-retardant nature of certain phosphinated materials. Such polymers find utility in a number of applications, including the electronics sector and soft materials. Phosphorus-based polymers exhibit a wide range of properties such as flame retardancy, mechanical properties, thermal stability, proton or anion conductivity, and anticorrosive resistance when compared with traditional organic or inorganic polymers [116].

ii. Organic polymers. Porous organic polymers have a porous framework that is impregnated in various dimensions. These polymers arise from covalent bonds between the organic monomers of different orientations and shapes. They can be categorized as crystalline or amorphous depending on the difference in the arrangement of monomers in their structure. They are mainly used as photocatalysts for modifications because of their extraordinary stability, inherent porosity, economical designs, and flexibility in structure and function. The nature, pore size, functions, and surface area of these polymers can be altered by modifying their side chains. They are used for heterogeneous catalysis, photocatalytic conversion, biochemical sensors, and gas and energy storage. There are different variations in their structure, so they could be divided into polymers that have homogenous catalysts, such as monomers; polymers that are altered post-synthesis; and polymers that have coordinated metal ions [112,117].

iii. Inorganic–organic hybrids. The coupling of inorganic materials with an organic polymer matrix produces inorganic–organic hybrid materials. Their mechanical, thermal, and physical properties are enhanced to a high extent. The strength of coupling between inorganic and organic depends on the conjugation with the polymer matrix, the number of particles, and the regular dispersal of particles in the 3D network. These polymers' thermoplastic or thermosetting behaviors and elasticity are improved by inorganic fillers [118]. This new family of polymer composites combining inorganic and organic systems is prepared in situ using sol–gel processes. By optimizing the conditions for their synthesis, their characteristics can be controlled. The inorganic constituents provide stability to heat and friction and enhance chemical and electromagnetic properties and the refractive index, while the organic components are responsible for producing films. Hybrid systems are improved compared to the individual constituents [112].

Conducting polymers belong to the family of conjugated polymers, which include polyaniline, poly(p-phenylene vinylene), polyethylene oxide, polypyrrole, poly(3,4-ethylene dioxythiophene), poly(2,2′ bithiophene), and polythiophene. They have been shown to be valuable materials in high-tech technologies, such as photocatalysis, sensors, biosensors, nanotechnology, and organic electronic devices [104,105].

Polyaniline (PANI) has been one of the most studied conducting polymers due to its numerous possible applications [119]. The terminology of a quasi-metal univocally designates its electronic properties [120]. PANI is an electrically conductive polymer that is easily prepared using chemical or electrochemical oxidation of aniline, usually in aqueous medium [121]. Due to its electrochemical, electrical, and optical properties and excellent thermal and environmental stability, it has emerged as one of the leading conducting polymers for photocatalytic commercial applications [122]. The main disadvantage of PANI is poor processability both in melt and solution processing as a consequence of its backbone stiffness [123]. PANI salt, emeraldine hydrochloride, is not soluble in common organic solvents. It is soluble only in concentrated sulfuric acid. However, recent discoveries have found that functionalized protonic acids like camphor sulfonic and dodecylbenzene sulfonic acid, together with phosphoric acid esters, enable polyaniline salts to dissolve in organic solvents [124]. PANI can have its physical properties precisely tailored to meet the requirements of various applications by applying several synthetic methods. The potential of the PANI thin film on conductive electrode surfaces as an efficient photocatalyst and the possibility of using it as a photocatalyst in different conjunctions have been studied by many authors [125–128]. In order to achieve suitable environmental and thermal stability, three doping forms of PANI have been designed using post-treatment oxidation methods. Newly synthesized PANI materials (emeraldine base, pernigraniline form, and leucoemeraldine base) have been studied by many characterization techniques such as SEM, TEM, EDS, EPR, XRD, XPS, DRS, and FTIR methods. The results of these studies revealed these materials' high photocatalytic activity in pharmaceutical degradation. The emeraldine base's low band gap, policrystallinity, and the fact that it possessed the most active sites made it the best candidate in comparison with the other two materials [129–133].

Poly(p-phenylene vinylene) (PPV) possesses long-term π-conjugation and photophysical properties, which are suitable for photocatalysis [134]. Moreover, the easy chemical modification and synthesis strategy of PPV can obtain various derivatives [135]. Therefore, PPV is a promising candidate for different applications like photocatalytic degradation, CO_2 reduction, H_2 production, and organic synthesis [136]. PPV is also an essential conjugated polymer used in various optoelectronic devices, such as solar cells, light-emitting diodes, organic transistors, and chemical sensors [134]. PPV-based materials exhibit both p and n doping properties. These materials can be oxidized in the positive potential range [137]. When the polaron is formed, the positive charge is delocalized over the average of the four monomer units. Also, oxidizing PPV units undergo disproportionation processes leading to the formation of localized dications, which are separated by four neutral monomer moieties. The PPV oxidation process is followed by the incorporation of supporting electrolyte anions into the polymeric network. Also, PPV and its derivatives can be reduced at negative potentials to form negative polarons and dope the polymeric phase with the cations of the supporting electrolyte [134]. PPV is utilized in a wide range of applications, including molecular imaging, light-emitting devices, biosensors, and anticancer therapy. Recently, there have been an increasing number of studies on the application of PPV-based materials in the field of photocatalysis [138–141]. When deposited on an appropriate material, PPV is able to significantly improve its photocatalytic response, allowing the controlled formation (or retention) of exciting matter [142]. PPV and its derivatives have been proven to be important photoactive components for fabricating polymer–inorganic hybrid nanocomposites, which can be easily processed into stable and efficient photoactive coatings that are almost exclusively responsive to visible light within the solar spectrum [138].

Polyethylene oxide (PEO). Hydrophilic polymers have been an essential class of materials for various applications as biocompatible and biodegradable materials [143]. PEO, also known as polyethylene glycol, is a polyether polymer that has recently received a great deal of attention in research and industrial applications in the area of photocatalysis [144]. PEO has been widely used due to its biocompatibility and non-toxicity properties. PEO is a very versatile polymer with a wide range of applications, such as solid polymer electrolytes [145]. As its name indicates, PEO has an oxide group within the main chain; therefore, it is possible to tailor the material according to the requirements of the intended application. The polymer features good dielectric and ion-related properties due to its structure, high solvation power, easy formation of complexes with alkali salts, and the fact that it provides a direct path for cation migration [146]. Considering complex materials design for advanced multifunctional materials for the most strategic sectors, it appears clear that the tailoring of PEO is fundamental for progress in the field of energy storage technologies, like fuel cells and batteries, as well as eco-sustainable solutions for the use of PEOs in water remediation technologies [147].

Polypyrrole (PPy) Electrically conducting polymers have received a considerable amount of attention due to their usability in different applications, such as field-effect transistors, light-emitting diodes, solar cells, and photocatalysis processes [148]. Electrically conducting polymers are amorphous or semi-crystalline organic compounds that exhibit metallic levels of electronic conductivity and high electrochemical and chemical stability, similar to inorganic semiconductors [149]. PPy is a nitrogen-containing five-membered heteroaromatic ring molecule [150]. Five lone-pair electrons are present on the nitrogen atom, which are beneficial for electron transfer, and hence, there is an easy and moderate oxidation of PPy to form PPy^+ [151]. This feature is advantageous for the modification and post-synthesis functionalization of the PPy. To improve the potential applications of doped PPy for ions from anionic environmental pollutants, some approaches to reversible tuning of the PPy^+ anion exchange membrane to PPy upon removal of the specifically adsorbed ions have been reported in the literature [152,153]. Changes in the electronic structure of PPy can be identified through spectroscopic and electrochemistry-based techniques. Thus, the solid-state near-edge X-ray absorption fine structure spectra revealed an increase in the occupation probability of the electronically conducting π electrons in the partially or fully oxidized PPy [154].

2.2. Modification of Polymers for Enhanced Photocatalytic Activity

The directed modification of synthetic polymers has long been known to significantly expand the range of polymer utility, even when only a few fundamental chemical transformations are available for this purpose [132]. Techniques for polymer modifications to enhance their photocatalytic activity are divided into physical and chemical modification techniques.

2.2.1. Physical Modification Techniques

Mechanical blending. Although a number of methods are available for the preparation of polymer blends, a common one is using a stirrable device in the liquid phase. It is called mechanical blending [155]. In a typical preparation, the polymers to be blended are mixed above the glass transition temperature of the polymers to allow proper mixing and obtain a homogeneous melt. Polymeric blends can also be used to meet requirements for various physical and mechanical characteristics, such as processability, abrasion resistance, impact resistance, and deformability, as well as to meet the needs of biocompatible and environmental formulations with higher biological activity. From these evaluations, toughened plastics, composite materials, films, fibers, elastomers, and gels can be prepared [156]. Therefore, the mechanical blending of polymers is crucial in improving polymers' properties for the purpose of removing pharmaceutical pollutants by the photocatalytic process. Blending polymers gives stable mixtures that have been used to create a variety of polymers with specific physical and chemical properties for use in some forms of processing. This is particularly attractive because it is generally less expensive to formulate blends than to synthesize entirely new polymers [157].

Extrusion processing. Extrusion and injection molding are widely used methods in polymer processing. In extrusion, polymer melts continuously in a conduit (barrel) and is subsequently forced through a restrictive forming tool. During the extrusion process, polymer melts and is transported through different geometries, takes a complex shape, cools down, and ultimately solidifies into the desired form. For the products of commercial polymers, crystallization usually happens during the extrusion process [158]. In the case of semicrystalline polymers, the most critical factors influencing the properties of the products can be cooling rate, temperature, pressure, and the orientation of the elongated macromolecular chains.

Moreover, extrusion is usually the final process in a complex macromolecular material technology involving operations like the crystallization of newly formed macromolecules [159]. As a result of limiting the operating conditions and the pressure drop in the system (especially at the die hole), the extrudate emerges as a solid, e.g., stock, a profile, a pipe, or a film. Obtained materials are widely used to remove pharmaceutical contaminants from the environment through adsorption or photodegradation. The high value of the die compression ratio means that the effective pressure drop in the die is also enhanced, leading to an increase in viscosity and then an increase in extrusion force [160]. A reduction in the die compression ratio leads to a reduction in the adequate pressure in the die and a correspondingly more significant decrease in viscosity. If speed decreases, a discontinuous flow of material can occur [161].

The ongoing evolution of computer technology has resulted in the ability to perform complex optimization studies on many aspects of single-screw profile extrusion, which would be uneconomical using predictive full 3D numerical simulations. As single-screw extrusion processes of polymer materials are susceptible to numerous influencing parameter combinations, an overall optimization of the distinct technical task is essential [162]. The steady-state computational approach based on a 3D solver has several drawbacks, e.g., computational time and resource use, especially for the simulation of thermal processes with defined temperature boundary conditions. The need for computational optimization to obtain new polymer materials will be illustrated with an example of injection stretch blow molding. The main process steps are illustrated in Figure 2a–f. An injection unit (Figure 2a) fills the cavity of an injection mold (Figure 2b) to produce a pre-form material. This is then transferred to a blow mold (Figure 2c), where it is stretched and blown (Figure 2d) against the contours of the mold cavity. The mold opens (Figure 2e) when the container is sufficiently cold. Modeling of this process to predict the performance of the part for a given set of input conditions (operating conditions, equipment geometry, material properties) typically entails the numerical modeling of each of its steps, followed by expensive process costs. Therefore, before the process starts, modeling the thickness, morphology, and mechanical performance of polymers and their action on pharmaceutical molecules could be predicted. It is suggested that the optimization process be approached backward, as indicated by the curved arrows (Figure 2, from 1 to 5) [159].

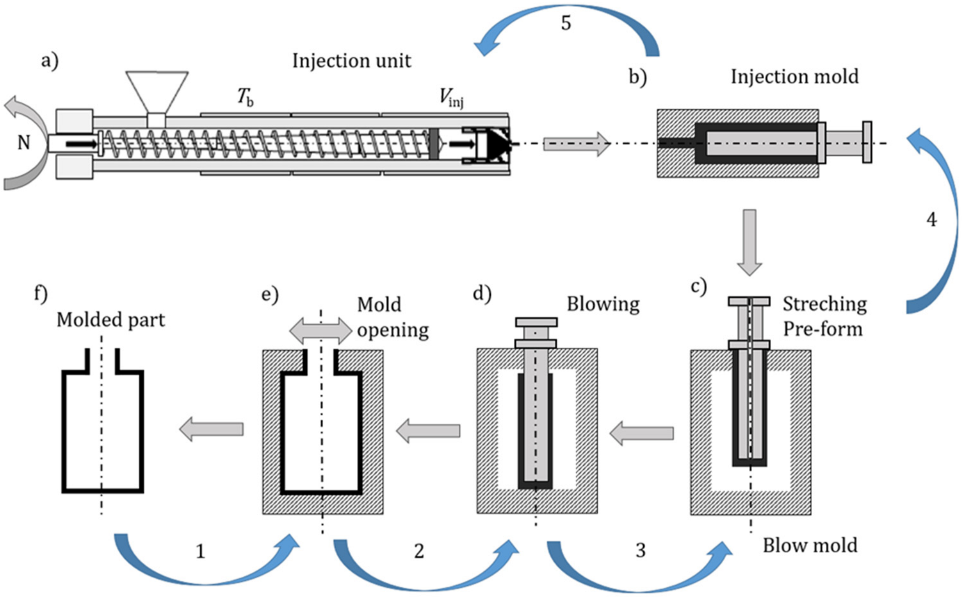

Figure 2. Optimization of injection stretch blow-molding. (**a**–**f**) illustrate the process steps. Straight arrows follow the process sequence; curved arrows follow the optimization sequence. N—screw speed, T_b—barrel temperature profile, V_{inj}—injection volume. Reprinted with permission from Ref. [159], copyright MDPI.

2.2.2. Chemical Modification Techniques

Nanocomposite formation. Interaction between a component of the polymer matrix and the nanoparticle surface can be an additional aspect that occurs during the production of classical composites by reinforcing the polymer matrix with filler. Such an interaction, in some aspects, limits the possibility of selecting the filler, significantly changing the internal structure of the polymer nanocomposite and affecting the properties of these materials in the removal of pharmacological compounds from the environment. Nanoparticle dispersion in the polymeric matrix is another essential aspect of research on polymer nanocomposites [163]. Polymer nanocomposites are an important class of materials that are popularly used in various applications due to their characteristic unique behavior in comparison to their pristine polymer forms [164]. The ability to control nanoscale particle dispersion can lead to unique properties (mechanical, electrical, and thermal properties) due either to molecular confinement or control over the structure formation process during nanocomposite production [165]. The most common applications of polymer nanocomposites are in photocatalysis, biomedicine, and other industrial applications [166–168].

The dispersion of the nanoparticles, their size, their surface topography, and the chemical properties of the interface with the polymeric matrix all together play an essential role in defining the characteristics of the nanocomposite [169]. These nanocomposites can have rheological, mechanical, and gas barrier properties that surpass the best traditional composites but often also have new functionalities like flame retardancy, transparency, light shielding, photocatalytic activity, or environmental sensors [170]. In the development of complex systems formed by nanoscopic inorganic clusters and organic matrices, it is essential to understand the architecture of the polymer matrix at the level of dynamic and static nanoscopic heterogeneity. In this field, a fundamental issue is to understand how the functional properties of a polymer change due to the complex nanoscale architecture of the matrix formed by the dispersed material [171].

Plasma modification. Process control and plasma generation are the main aspects of polymer modification in many applications, including nanotechnology, material science, and biomedical engineering [172]. The generation of plasma is achieved by the application of an electric field to typically an inert gas, leading to the ionization and excitation of gas molecules. Created plasma is a highly reactive mixture of radicals, electrons, ions, and excited species [173]. To achieve effective polymer modification, control of the plasma generation process and parameters such as exposure time, gas flow rate, power, and pressure are essential. Properties of the plasma, such as its composition, temperature, density, and ultimately the modification of the material surface, can be significantly affected by these parameters [174]. Plasmas offer multiple ways to modify polymer surfaces and thus influence the adhesion environment. Polymer substrates benefit from direct interaction with the plasma medium, and impinging charged and neutral plasma species acquire an organization fitting within two physical processes of interaction, i.e., the formation of permanent polar/aromatic groups or the grafting of other chemical functions via intermediate activation sites [175]. These chemical modifications can affect the polymeric network, generally reducing hydrophobicity and replacing aliphatic molecular moieties with new anchoring points for further chemical surface tailoring [176]. Many techniques are used to generate plasma, such as radiofrequency, alternating current, and direct current. The choice of technique depends on the desired surface properties of the material being modified. For example, radiofrequency plasma is commonly used to modify polymers and remove pharmaceutical compounds through photocatalytic processes [177].

Surface functionalization. Surface functionalization refers to any chemical reaction that alters the surface of a material, or modifies or introduces physicochemical properties without fundamentally changing the bulk characteristics [178]. A properly designed surface can be implemented using various direct surface functionalization processes. The most often used techniques are physisorption and chemisorption of small molecules and manufacturing composite materials [179]. Controlling the surface properties of materials is an essential factor in determining interactions between obtained materials and the environment. The first requirement for surface modification of materials is the introduction of new functionality and physical properties. Surface modification can be performed through various methods like surface-initiated polymerization, high-energy irradiation, and direct immobilization of natural entities [180]. Stereoregular polymers may be produced from optically active monomers. For example, in terms of salient features, chiral polymer production in either a racemic or a scalemic manner may lead to asymmetric surfaces with congruent properties. Another possibility lies in the use of optically active initiators directing the polymerization propagation processes towards the canonical synthesis even of atactic polymers [181]. Fluorescent, electronically active polymers are largely heterogeneous, including the strongly delocalized radical along the polymer chain. These are produced by overcoming the disadvantages of post-deposition functionalization techniques with their confined degree of grafting. Polymer incorporation into a material phase leads to significant changes in the properties of the surface, such as wettability, charge density, or even spatial distribution of functional groups. Various industrial applications are described in the literature: water purification, packaging in pharmaceutical and food industries, wood coatings for protection against sunlight, membranes for gas separation, coatings for textiles and optical sensors, optical information storage, soft contact lenses, etc. [182–184].

Cross-linking. Some of the polymers used in composite systems, photocatalytic processes, and other applications are thermoset or cross-linked polymers [185]. Cross-linking polymers containing one or more reactive monomeric subunits can produce materials with three-dimensional net points connected by covalent bonds in a process that is often referred to as curing. Various covalent reactions are used to cross-link polymers, many of which can be considered “click” reactions because they are efficient, regiospecific, and lead to high conversions [186,187]. In particular, they can be used to create environmentally robust, mechanically tough, and heat-resistant materials. By controlling those properties, new materials with unprecedented functionality are expected to emerge, enabling different applications such as all-polymer actuators and novel optical devices. In the last few years, many polymers based on dynamic covalent bonds have been modified and used in many fields because of their superior properties [188,189]. Polymers obtained by cross-linking, with shear self-repairing and thinning properties, are often used in 3D printing, and polymers with antibacterial, conducting, and self-healing properties are often used in photocatalytic reactions [190].

3. Efficiency in Removing Pharmaceutical Pollutants

Photocatalysis is a chemical reaction in which the catalyst is activated by light. Catalysts accelerate a chemical reaction by lowering the activation energy, making the reaction easier. In a conventional chemical reaction, heat is commonly used to activate catalysts. Photocatalysis provides an alternative way to carry out reactions at a reduced temperature, therefore decreasing side products that may be formed. Overall, this yields increased economical and environmentally friendly reactions. The field of photocatalysis has made significant progress, replacing several conventional methods based on its cost-effectiveness and utility [191]. The general mechanism of photocatalysis is based on the use of a semiconductor, which enables the absorption of visible or UV light from the solar spectrum. Absorption of irradiation causes the excitation of electrons from valence band to conduction band and generates e^-–h^+ pairs. In the next step, e^- and h^+ are transferred to the photocatalyst surface for the degradation and oxidization of pollutants to CO_2 and H_2O [192].

In general, the photocatalysis process involves three significant steps: photocatalyst light absorption, separation of photogenerated charge carriers, and interfacial catalytic redox reactions [193]. When the conducting polymer is irradiated with UV/Visible light, an e^- from the valence band is excited by a photon of light to the conduction band. This phenomenon is called π-π^* electronic transition. The excited e^- migrates to the surface of the conducting polymer and activates the adsorbed O_2 molecules to form superoxide radicals $O_2^{\bullet -}$, which oxidize organic contaminants in the aqueous environment (Figure 3a). Photogenerated h^+ can also oxidize organic pollutants directly [194]. In the case of conducting polymer–metal oxide hybrid (Figure 3b), conducting polymer acts as a photosensitizer, and it is able to absorb a wide range of visible irradiation because of the lower band gap compared to metal oxide. The excited e^- in the lowest unoccupied molecular orbital (LUMO) of conducting polymer chains is injected into a conduction band of transition metal oxide (e.g., TiO_2, ZnO), which reacts with an adsorbed water molecule to form $O_2^{\bullet -}$ radicals. h^+ can react with water to form $HO^\bullet$. These polymer modifications, with improved photocatalytic activity, are widely used in the degradation of pharmaceutical compounds by the photodegradation process [81,105].

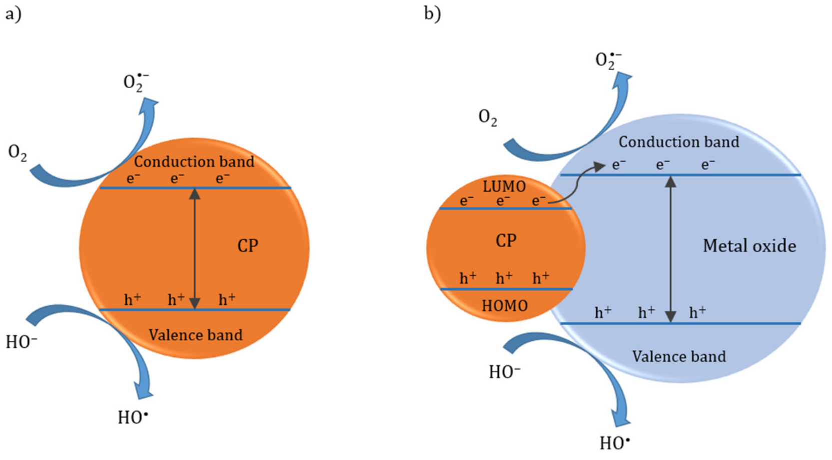

Figure 3. The scheme of photocatalysis, based on a (**a**) conducting polymer (CP) nanocomposite and (**b**) conducting polymer–metal oxide hybrid modification. Reprinted and adjusted with permission from Ref. [192], copyright MDPI.

Researchers are taking a greater interest in the development of new polymeric materials that have a high affinity for harmful organic compounds and also exhibit high fluxes in membrane separation processes for the treatment of natural water, underground, and domestic and industrial sewage. Polymers and polymer-based structures have found a wide range of applications in the removal of pharmaceuticals from the environment [195,196]. Discussions on this topic have been recognized since around 2000. Since the year 2000, 5616 articles related to the use of polymers in photocatalysis have been published, while only 128 articles have referred to the photocatalytic degradation of pharmaceuticals by the use of polymers as catalysts [197]. The main aim of the present work was to comprehensively address studies performed using polymers to achieve effective removal of pharmaceutical contaminants from the environment.

The high synergy between PANI and ZnO was observed by Nosrati et al. [198]. They used PANI/ZnO to remove ampicillin. It was indicated that PANI/ZnO composites could be reused multiple times with a minimal loss of reactivity. ZnO/PANI nanocomposite was also synthesized by Asgari et al. [199] and used in the photocatalytic degradation of metronidazole. The photocatalytic activity of the ZnO/PANI nanocomposite in the degradation of MNZ was 63 times higher than that of ZnO under visible light radiation. Šojić Merkulov et al. [200] investigated the kinetics of photocatalytic degradation of pharmaceuticals in the presence of TiO_2/PANI nanocomposite powders. Degradation and mineralization efficiency of propranolol and amitriptyline using TiO_2/PANI was high in environmental waters.

The synergistic association of WS_2/PANI nanocomposite can degrade pollutants such as antibiotics (nitrofurantoin). This research was conducted by Fatima et al. [201], wherein the WS_2/PANI nanocomposite was successfully synthesized via a facile, in situ polymerization technique. By using the in situ oxidative polymerization method, Ujwal et al. [202] synthesized $GdFeO_3$/PANI nanocomposite. The chemical, physical, and structural properties of $GdFeO_3$/PANI enabled electrochemical detection and photocatalytic degradation of an organic pollutant, acetaminophen. Tahir et al. [203] synthesized a novel nanocomposite of Bi_2WO_6 through PANI intercalation. This nanostructure exhibited effective charge separation and outstanding activity in hydrogen evolution and photocatalytic degradation. Fabricated nanocomposite showed higher stability even after four degradation cycles. PANI/$LaFeO_3$/$CoFe_2O_4$ ternary heterojunction was synthesized by in situ polymerization by Kumar et al. [204]. In comparison with the photocatalyst PANI, the synthesized PANI/$LaFeO_3$/$CoFe_2O_4$ was shown to be superior. It led to degradation of 92% of the selected pharmaceutical after 120 min of irradiation.

Dai et al. [205] synthesized 3D PANI/Perylene diamide and applied it in pharmaceutical removal using visible irradiation. They provided a promising approach for improving the photocatalytic performance of polymer materials and indicated that 3D PANI/PDI organic heterojunction can be efficiently applied for water treatment remediation. PANi@carbon nanotubes/stainless steel was designed by Peng et al. [206]. Synthesized material showed high efficiency, was environmentally friendly, and stable. It was used and proved to be effective in the degradation of pharmaceutical ibuprofen. Tian et al. [207] synthesized carbonized PANI-activated peracetic acid and used it in the degradation of different pharmaceutical compounds. A high degradation rate of pharmaceuticals was observed, while the primary reactive species for degradation was $HO^{\bullet}$.

Table 2 represents a summary of PANI composites used for photocatalysis of pharmaceutical compounds.

Table 2. Photocatalysis of pharmaceuticals using PANI composite materials.

Type of Polymer Composite	Synthesis of Photocatalyst	Contaminant	Light	Removal Efficiency (%)	Lamp Power	Reference
ZnO/PANI nanocomposite	Chemical adsorption	Ampicillin	Sunlight	41% in 120 min	-	[198]
ZnO/PANI nanocomposite	In situ chemical polymerization	Metronidazole	Visible	97% in 180 min	300 W Xenon lamp	[199]
TiO_2/PANI nanocomposite	Oxidative polymerization	Propranolol	UV irradiation	34% in 60 min	125 W High-pressure mercury lamp	[200]
TiO_2/PANI nanocomposite	Oxidative polymerization	Amitriptyline	UV irradiation	45% in 60 min	125 W High-pressure mercury lamp	[200]
WS_2/PANI nanocomposite	In situ polymerization	Nitrofurantoin	Visible	99% in 120 min	Xenon arc lamp	[201]
$GdFeO_3$/PANI	In situ oxidative polymerization	Acetaminophen	Visible	88% in 60 min	30 W Light emitting diode	[202]
Bi_2WO_6/PANI	Intercalation	Ciprofloxacin	Visible	98% in 90 min	50 W Halogen lamp	[203]
PANI/$LaFeO_3$/$CoFe_2O_4$ ternary heterojunction	In situ polymerization	Clozapine	Visible	92% in 120 min	50 W Halogen lamp	[204]
3D PANI/Perylene diimide	In situ growth	Tetracycline	Visible	70% in 120 min	5 W LED lamp (420 nm cut-off filter)	[205]
PANi@carbon nanotubes/stainless steel	In situ polymerization	Ibuprofen	Visible	76% in 35 min	300 W Xenon lamp	[206]
Carbonized PANI-activated peracetic acid	Interfacial polymerization	Sulfamethoxazole	Visible	100% in 60 min	30 W Light emitting diode	[207]
Carbonized PANI-activated peracetic acid	Interfacial polymerization	Naproxen	Visible	100% in 60 min	30 W Light emitting diode	[207]
Carbonized PANI-activated peracetic acid	Interfacial polymerization	Antipyrine	Visible	30% in 60 min	30 W Light emitting diode	[207]

PPy-based composites also exhibit significant photocatalytic properties in pharmaceutical degradation. Silvestri et al. [208] applied PPy-ZnO synthesized via polymerization in the degradation of diclofenac. The PPy-ZnO was demonstrated to be highly active for diclofenac degradation under simulated solar irradiation, even when compared with pure ZnO. Jiadi et al. [209] synthesized TiO_2@V_2O_5-PPy, exhibiting high photocatalytic performance and water stability. This photocatalyst has been used to remove water-soluble organic pollutants with high efficiency under visible light irradiation. The photocatalytic degradation ability of the newly synthesized Fe-TiO_2-PPy was investigated under solar light. From the results, it can be concluded that the prepared Fe-TiO_2-PPy could be an efficient adsorbent as well as a photocatalyst for the degradation of pharmaceuticals from an aqueous environment [210].

Ultrasound-assisted synthesis of PPy/V_2O_5 was performed by Zia et al. [211]. The obtained photocatalyst was used in the visible-light-driven photodegradation of erythromycin and ciprofloxacin. The generation of hydroxide and superoxide radicals was enhanced by the use of a newly synthesized composite. Kumar et al. [212] synthesized Fe_3O_4 nanorods coated in PPy/rGO by a chemical reflux method. Fe_3O_4@PPy/rGO showed good repeatability, stability, and reproducibility. Photocatalytic studies revealed 84% degradation of acetaminophen by Fe_3O_4@PPy/rGO in the presence of persulfate. Zhu et al. [213] successfully synthesized high-dispersed PPy@Ag/g-C_3N_4. The as-prepared PPy@Ag/g-C_3N_4 was used to remove various organic pollutants from the water. It was established that enhanced photocatalytic activity of PPy@Ag/g-C_3N_4 came from π-conjugated electronic structures of PPy and Ag species as well as the electron transfer mediator between g-C_3N_4 and PPy.

The newly synthesized nanocomposite Ag_2MoO_4/PPy performs as an efficient photocatalyst in the degradation of pharmaceutical ciprofloxacin within 10 min. As prepared, Ag_2MoO_4/PPy provided a defined morphology, larger surface area, and smaller size, and this improved its electrocatalytic and photocatalytic properties [214]. Das et al. [215] fabricated new PPy-sensitized zinc ferrite/graphitic carbon nitride by an in situ polymerization method. This material showed good photocatalytic performance towards ciprofloxacin degradation and generation of hydrogen energy. It may offer a promising strategy for maximum light absorption that meets environmental claims.

Table 3 represents a summary of PPy composites used for photocatalysis of pharmaceutical compounds.

Table 3. Photocatalysis of pharmaceuticals using PPy composite materials.

Type of Polymer Composite	Synthesis of Photocatalyst	Contaminant	Light	Removal Efficiency (%)	Lamp Power	Reference
PPy-ZnO	Polymerization	Diclofenac	UV and visible	81% in 60 min	Xenon lamp (wavelength range 250–800 nm)	[208]
TiO_2@V_2O_5-PPy	In situ polymerization	Tetracycline	Visible	98% in 120 min	300 W Xenon lamp	[209]
TiO_2@V_2O_5-PPy	In situ polymerization	Doxycycline	Visible	96% in 120 min	300 W Xenon lamp	[209]
TiO_2@V_2O_5-PPy	In situ polymerization	Oxytetracycline	Visible	85% in 120 min	300 W Xenon lamp	[209]
Fe-TiO_2-PPy	Polymerization	Tetracycline hydrochloride	Sunlight	96% in 180 min	-	[210]
PPy/V_2O_5	Ultrasound-assisted synthesis	Ciprofloxacin	Visible	53% in 50 min	300 W Xenon arc lamp	[211]
PPy/V_2O_5	Ultrasound-assisted synthesis	Erythromycin	Visible	76% in 50 min	300 W Xenon arc lamp	[211]
Fe_3O_4@PPy/rGO	Chemical reflux	Acetaminophen	UV and visible	84% in 120 min	250 W tungsten-halogen	[212]
PPy@Ag/g-C_3N_4	Calcination followed by surface polymerization	Danofloxacin	Visible	90% in 60 min	300 W Xenon lamp	[213]
PPy@Ag/g-C_3N_4	Calcination followed by surface polymerization	Tetracycline	Visible	95% in 60 min	300 W Xenon lamp	[213]
PPy@Ag/g-C_3N_4	Calcination followed by surface polymerization	Ciprofloxacin	Visible	92% in 60 min	300 W Xenon lamp	[213]
PPy@Ag/g-C_3N_4	Calcination followed by surface polymerization	Gatifloxacin	Visible	89% in 60 min	300 W Xenon lamp	[213]
PPy@Ag/g-C_3N_4	Calcination followed by surface polymerization	Enrofloxacin hydrochloride	Visible	91% in 60 min	300 W Xenon lamp	[213]
Ag_2MoO_4/PPy	In situ synthesis	Ciprofloxacin	Sunlight	100% in 10 min	-	[214]
PPy-sensitized zinc ferrite/graphitic carbon nitride	In situ polymerization	Ciprofloxacin	Visible	92% in 120 min	300 W Xenon lamp	[215]

Besides photocatalytic activity, polymer materials are also used as adsorbents for the efficient removal of pharmaceuticals. The potential and structure of polymeric adsorbents are of much interest in the context of understanding the adsorption phenomenon in solid materials [216–218]. The sorption curve or the adsorption isotherm is the most general way to describe the adsorption capacity of the adsorbent or the amount of the adsorbate adsorbed. The specific surface area of polymer materials is the most important parameter characterizing the porous structures of the adsorbent [219]. It is related to the adsorption capacity. In addition, the thermodynamics of the adsorption process are still of great interest, including the enthalpy of adsorption, entropy, and free energy change accompanying the adsorption process. These have provided valuable insight into the adsorption mechanism at the molecular level. Furthermore, the adsorption mechanism of the adsorbent toward the pharmaceuticals in water can be better understood by detecting the surface groups and information about the interactions between the specific groups of the pharmaceutical molecule and the functional ligands on the polymer [220,221].

4. The Role of Atomistic Calculations in Polymer-Assisted Photocatalytic Degradation

The term "atomistic calculations" encompasses a variety of theoretical and computational methods used to perform simulations on molecular and periodic structures. Other names for this class of theoretical tools are molecular modeling, computational chemistry, computational physics, etc. Over the last two decades, scientists have been able to predict a vast number of properties at the atomic level using these calculations and simulations, which are now possible to perform even on simple personal computers [222–224]. Atomistic calculations include methods such as molecular dynamics (MD) simulations, ab initio calculations, density functional theory (DFT), semiempirical calculations, and molecular docking, among others [225–227]. These techniques allow researchers to study the behavior of materials, predict their properties, and understand complex processes at an unprecedented level of detail. Advancements in computational power and the development of sophisticated algorithms have made it feasible to tackle problems that were once considered highly challenging, leading to significant breakthroughs in materials science, chemistry, and nanotechnology [228].

The power of atomistic calculations is best illustrated by the fact that the first step in the development of novel materials or the improvement of current ones often involves the application of computational methods to predict the properties of structures before they are synthesized. This approach allows researchers to identify the best candidates for physical experimentation, thereby optimizing research and minimizing the use of resources. By using these computational techniques, scientists can efficiently screen a wide range of materials and focus on those with the most promising properties, significantly reducing the time and cost associated with experimental trials. This predictive capability is a fundamental part of modern materials science and engineering, driving innovation and accelerating the discovery of advanced materials.

Over the years, a vast array of methods has been developed for performing calculations on molecules. Nevertheless, three distinct directions of development have emerged, each with its own set of advantages and disadvantages. These methods often intersect and complement each other, forming a comprehensive toolkit for molecular simulations. Their relationships are illustrated in the Venn diagram presented in Figure 4.

In terms of computational modeling, polymers are most frequently treated as molecules rather than periodic structures, so we will refer to molecular calculations hereafter. In general, all basic computational methods for simulations of molecules can be divided into three main groups: classical mechanics, quantum mechanics, and semiempirical methods. Classical mechanics treats molecular systems as classical systems, where a molecule is observed as a collection of balls interconnected with springs. The balls represent atoms, while the springs represent bonds between atoms. This approach utilizes a "force field" to describe the potential energy of the system. Although this approach is relatively simplistic, it is very useful, especially if the equations used to calculate the total energy of a molecule are adequate. However, to derive accurate equations, it is necessary to parameterize the force field using data from a large number of molecules [229].

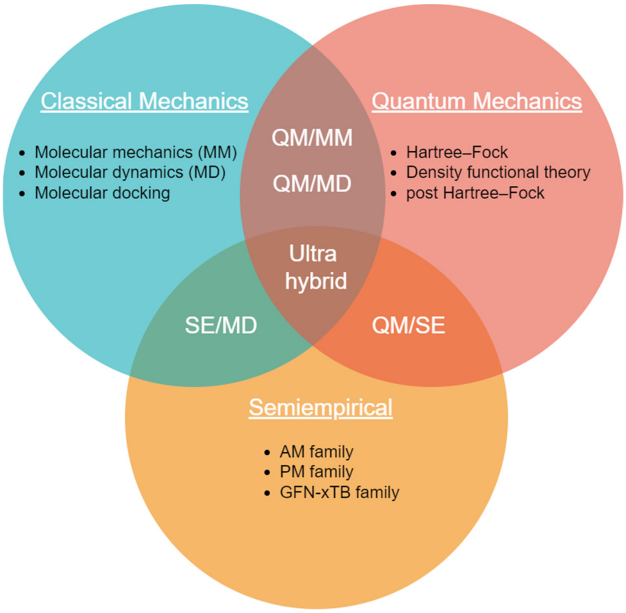

Figure 4. Venn diagram illustrating the connections between distinct computational methods for molecular simulations.

Quantum mechanical methods offer unprecedented accuracy for theoretical methods, but they come with a significant computational cost. Among these methods, one of the earliest was the Hartree–Fock (HF) method. This method is a typical example of wavefunction methods, meaning that the main task is to find a wavefunction that minimizes the energy of a given system. The main drawback of this method is that it does not account for electron correlations, which is where the density functional theory (DFT) method comes in. DFT is based on electron density, and the main task is to find the electron density that minimizes the energy of a molecule. This method accounts for electron correlation and is by far the most frequently applied computational method for calculations on molecules since it offers the best cost–accuracy ratio. DFT relies on the density functional, a function that determines how the energy of a molecule is calculated. However, based on the fundamental setup of DFT, there is no single, universal density functional suitable for all types of molecules. Literally hundreds of density functionals have been developed so far, and it takes experience to know which functional to apply and when. However, the best-known functional for calculations on molecules is undoubtedly the famous B3LYP [230–233], while for periodic structure, the best-known functional is certainly the PBE [234]. Post-HF methods offer unprecedented accuracy when it comes to various molecular properties; however, the computational costs associated with these methods prevent them from being applied to a higher extent, compared to DFT methods.

In the last decade, significant effort has been invested in the development of semiempirical methods. These methods are essentially quantum mechanical methods, but with additional approximations in the description of electron density and numerical procedures. For a long time, the parametrized method (PM) family of semiempirical methods [235–238] was the best choice. However, since 2017, the extended tight binding (xTB) methods developed by the renowned Professor Stefan Grimme and his group have emerged. In many significant aspects, these methods have achieved DFT accuracy at a fraction of the computational time required for calculations. Another important thing to mention is the fact that the GFN family of methods is available in the program called xtb [239–243], completely open source and free to use.

Currently, the latest xTB method is GFN2 [239], and aside from its remarkable accuracy, the superiority of this method over other semiempirical methods lies in its ability to cover the majority of the periodic table of elements (PSE). The parameters for these semiempirical calculations are available for atoms with Z equal up to 86. In terms of xTB methods, the development of GFN methods has also led to the creation of the force field called GFN-FF. This force field stands out not only for its accuracy and speed but also for its automated applicability to the PSE, meaning that the only requirement to run it is the starting molecular structure.

There is a reason why we have devoted significant space to semiempirical methods, particularly to GFN-xTB methods. Polymers are large and highly flexible molecular structures, and their optimization via DFT methods can be quite demanding in terms of computational time. Additionally, highly rotatable functional groups can make vibrational analysis particularly difficult, making it very challenging to identify the ground-state geometry of the polymer chain. In such situations, we warmly recommend a multiscale modeling workflow, i.e., the application of different computational methods (Figure 5).

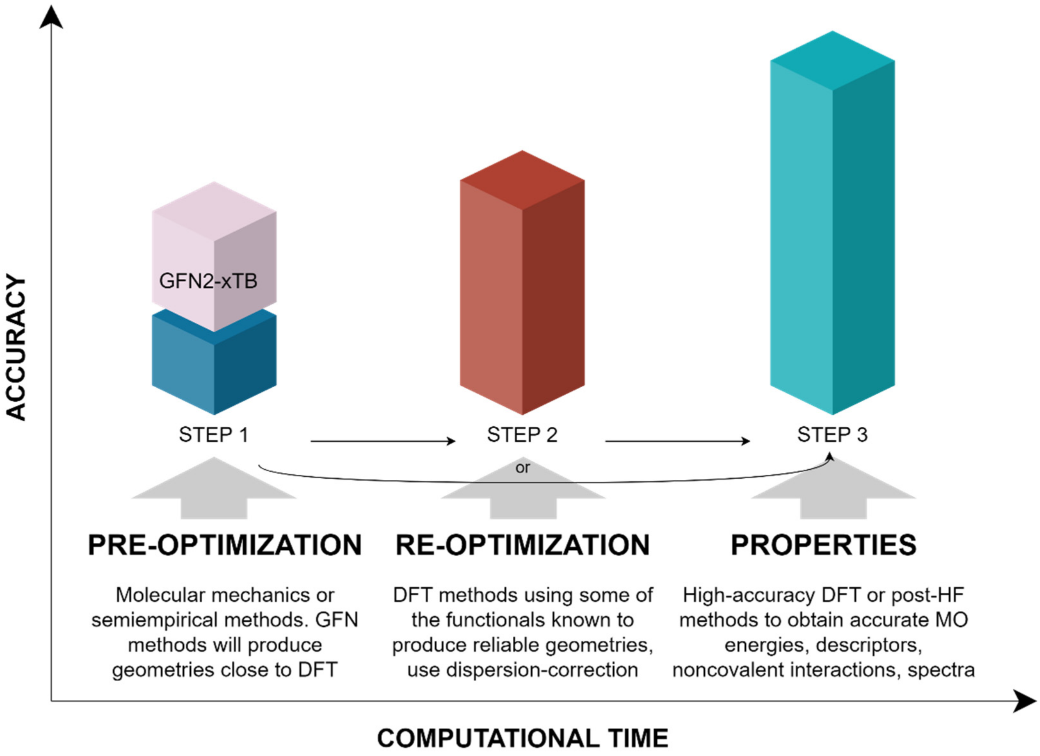

Figure 5. Suggested workflow for geometrical optimization and property calculations of long polymer chains.

To achieve faster geometrical optimizations, it is wise to pre-optimize large structures using very fast methods such as GFN2-xTB. This method yields optimized geometries that are very close to those obtained via DFT methods (Figure 6). Ground-state geometries obtained via GFN methods can be further re-optimized with DFT methods. This subsequent optimization is much faster since the pre-optimized structure is already very close to the ground state. This multiscale modeling approach significantly reduces computational time while maintaining high accuracy in the final optimized structures [244].

In Figure 6, we visually compare the optimized geometries of a polymethylmethacrylate (PMMA) polymer chain (consisting of five monomer units) obtained via the GFN2-xTB semiempirical method and the DFT method using the B3LYP-D3 density functional with the 6-31G(d,p) basis set. Both structures appear very similar, with no clearly visible differences in ground-state geometries. However, the GFN2-xTB method took less than five seconds for geometrical optimizations, while the DFT optimization at the specified level took almost two hours.

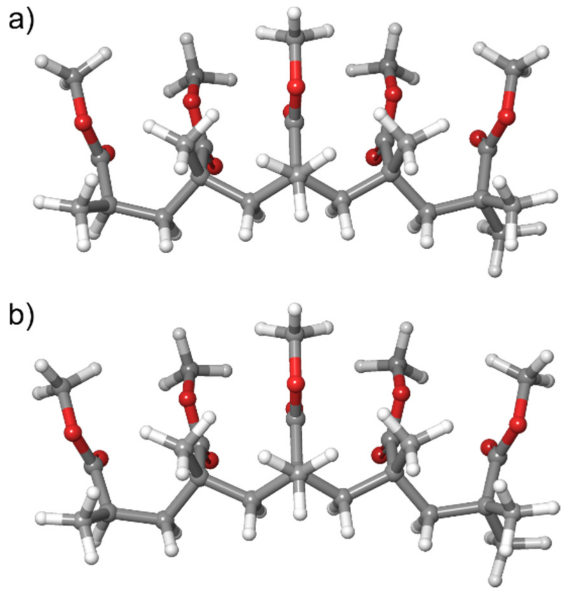

Figure 6. PMMA optimized via (**a**) GFN2-xTB and (**b**) B3LYP-D3/6-31G(d,p). Gray spheres represent carbon atoms, white spheres represent hydrogen atoms, red spheres represent oxygen atoms.

In the case of very large structures, ground-state geometries obtained via GFN methods can be treated as true ground-state geometries and further subjected to more accurate single-point energy calculations. This approach helps to obtain precise electron distribution, various quantum-molecular descriptors, spectral properties, non-covalent interactions, and more. Such a workflow is illustrated in Figure 5, demonstrating the efficiency and accuracy of combining GFN methods with single-point energy calculations for comprehensive molecular analysis.

One of the most powerful aspects of atomistic calculations in the context of photocatalytic polymers is the ability to estimate light absorption and charge transport properties. These crucial aspects of polymers' photocatalytic properties can be addressed with molecular orbital theory or time-dependent DFT (TD-DFT) calculations. Accurate DFT or post-HF calculations on geometrically optimized polymer chains yield the energies of the highest occupied and the lowest unoccupied molecular orbitals, HOMO and LUMO, respectively. The energies of these orbitals play a vital role in estimating reactivity and light absorption. The larger the energy gap, the less reactive the molecule, as a larger amount of energy is required to promote electrons from the HOMO to the LUMO. When combining polymers with photocatalytic nanomaterials, it is also important to know the "positions" of the polymers' HOMO and LUMO orbitals to find compatible combinations of polymers and photocatalytic materials [245].

In terms of improving photocatalytic properties, polymers are frequently used to achieve light sensitization of photocatalytic nanomaterials. In such cases, it is crucial to know the UV/Vis absorption spectrum of a polymer. While UV/Vis spectra can be inexpensively and quickly obtained experimentally, it is necessary to have the polymer physically first. However, synthesizing new structures is often complicated and expensive, making it beneficial to predict the UV/Vis spectrum prior to synthesis to select the best candidates. In this regard, TD-DFT calculations are extremely valuable, as they enable researchers to study excitations and construct UV/Vis spectra. A good illustration of how DFT methods can be applied for comprehensive computational studies of structural, reactive, and optoelectronic properties of polymers can be found in [246–249].

Regarding computational methods for studying polymers and other molecular structures, it is useful to mention modeling codes and packages currently available. Thanks to the amazing development of both computational codes and computer resources, researchers nowadays have a plethora of computational tools, most of which can be used on simple desktop computers. Computational codes for atomistic calculations can be either open-source, free-for-academics, or commercial [250].

Among open-source solutions, the xtb program of Professor Grimme and coworkers is an amazing tool with extensive possibilities for semiempirical calculations. This and other tools from this group are freely available on the official GitHub page of the Grimme group [251]. In addition to its remarkable functionality, the xtb program is also characterized by very detailed documentation with plenty of tutorials and case studies freely available [252]. Users are also warmly encouraged to visit the official web presentation of the Grimme group to learn more about computational tools and publications arising from them [253].

Online and desktop graphical user interfaces for the xtb program are available within the atomistica.online project. Atomistica.online is a free molecular modeling platform offering online and desktop tools for atomistic calculations, available at atomistica.online. One of the tools is the online GUI for the xtb program, allowing users to run most xtb calculations on a remote server through their web browsers for free. The current limitation is a molecule size of up to 200 atoms, which is sufficient for teaching and most research tasks. Tasks such as molecular dynamics simulations that cannot be run with the online tool can be easily run through the recently developed desktop xtb GUI. The desktop GUI for xtb removes the necessity of running the xtb from the command line and generating running commands or input files [254,255].

Regarding quantum mechanical calculations, the ORCA [256–264] code stands as one of the most powerful codes available. It is free for academics and can be obtained through the official forum [265]. This code, developed by Professor Frank Neese and colleagues, implements the latest DFT and wavefunction methods and is interconnected with the xtb code, making it a unique solution on the market. ORCA is well-documented, with plenty of tutorials and case studies, and features user-friendly input file structures. Another tool within the atomistica.online platform is the online input generator, a GUI for easy and user-friendly generation of input files for the ORCA modeling package. Atomistica also offers a desktop GUI for simple running and monitoring of ORCA calculations. All atomistica.online desktop tools are available for both Windows and Linux operating systems [264].

Since surface modifications with polymers play an important role in the functionalization of photocatalytic nanomaterials for water purification, we also mention the possibility of applying a combination of semiempirical and quantum mechanical calculations to study non-covalent interactions between a polymer and photocatalytic material. A detailed analysis of electron density within the molecular system is crucial for this purpose. The famous Multiwfn code [266], developed by Professor Tian Lu and freely available at its official web presentation [267], is extremely useful for this analysis and a vast number of other activities. By examining electron density between atoms, it is possible to identify specific sites where non-covalent interactions are formed and obtain information about their strengths. In particular, the concept of reduced density gradients (RDG) is very useful for this purpose. This approach allows for the identification of areas with specific electron densities indicating attractive or repulsive interactions between atoms [268]. Additionally, with the help of the Multiwfn program, it is possible to obtain RDG scatter plots and RDG surfaces, as shown in Figure 7.

The aforementioned RDG figures help researchers visualize the relationship between electron density and the reduced density gradient to identify non-covalent interactions and regions of weak interactions in a molecular system. The RDG scatter plot, presented in Figure 7a, represents specific points in space within a molecular system, each characterized by its electron density and reduced density gradient values. These dots help identify and visualize regions of non-covalent interactions, such as hydrogen bonds, van der Waals forces, and steric repulsions, by highlighting areas with low density gradients and varying electron densities. For example, a higher number of blue dots indicates a higher number of attractive non-covalent interactions. Similarly, the RDG surface, presented in Figure 7b, represents regions in three-dimensional space where the RDG values indicate the presence of non-covalent interactions. It is color-coded to show the nature and strength of these interactions based on the electron density values.

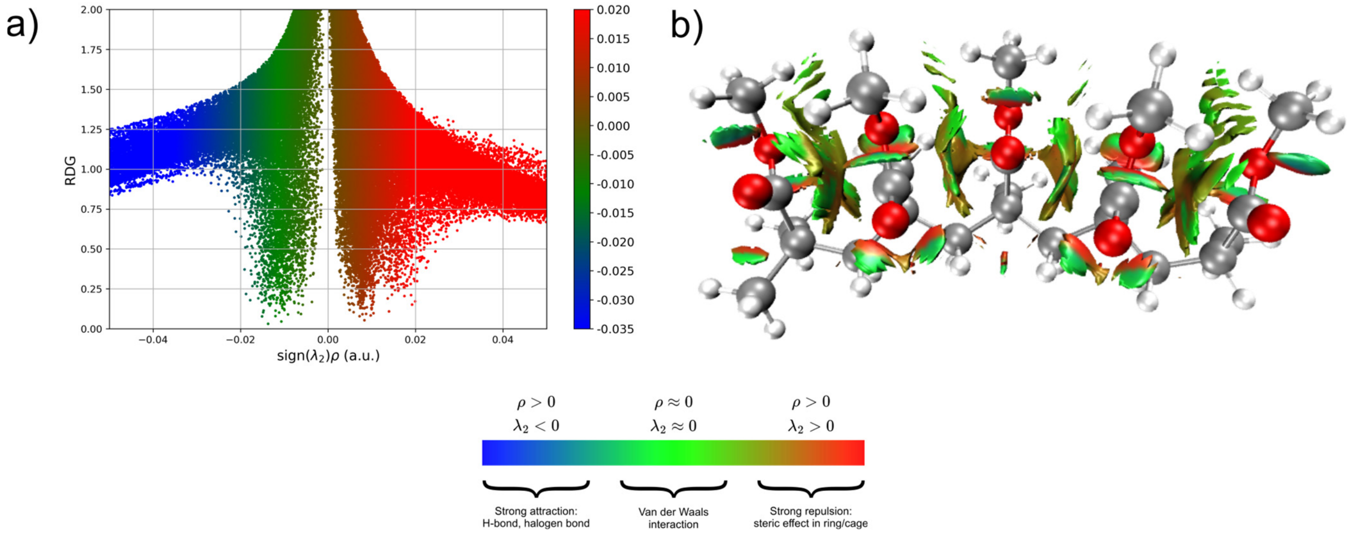

Figure 7. (**a**) RDG scatter plot and (**b**) RDG surfaces of PMMA polymer chain.

The atomistica.online project also offers an online tool for easily obtaining RDG scatter plots and files necessary to produce high-quality RDG surfaces through its user-friendly GUI, which runs Multiwfn in the background on a remote server provided by the project developers. Instead of working in the command prompt and combining several programs, users can easily obtain RDG scatter plots and files for RDG surfaces by simply uploading the output file containing the necessary information obtained after quantum mechanical calculations, for example, with ORCA [268].

Commercial solutions come at a price that can be quite high, but the graphical user interfaces, code optimization, and suites of tools for system preparation and data analysis justify the cost and enable users to achieve remarkable productivity. In terms of polymers, the commercial solution offered by Schrödinger, Inc. (New York, NY, USA) [269] within the Materials Modeling Suite [270] provides extremely useful tools for the preparation of polymer systems for quantum mechanical calculations and MD simulations, for running state-of-the-art classical and quantum mechanical calculations, and for the analysis of the obtained data and machine learning. This comprehensive tool enables researchers to study the intrinsic properties of polymers and interactions with photocatalytic materials through both molecular and periodic DFT calculations, allowing them to obtain, for example, band gaps of polymer-functionalized photocatalytic materials, which is of supreme importance for developing novel materials and procedures for water purification. Readers are warmly encouraged to study the case studies and documentation on the corresponding page of the Schrödinger, Inc. website [271].

5. Advantages and Challenges

As already pointed out throughout this manuscript, the use of photocatalytic polymers in the removal of pharmaceuticals from water has drawn significant attention due to their potential for efficient and sustainable water treatment. This chapter explores the advantages and challenges associated with this innovative approach. The benefits of the application of polymers in this area are summarized in the illustration presented in Figure 8.

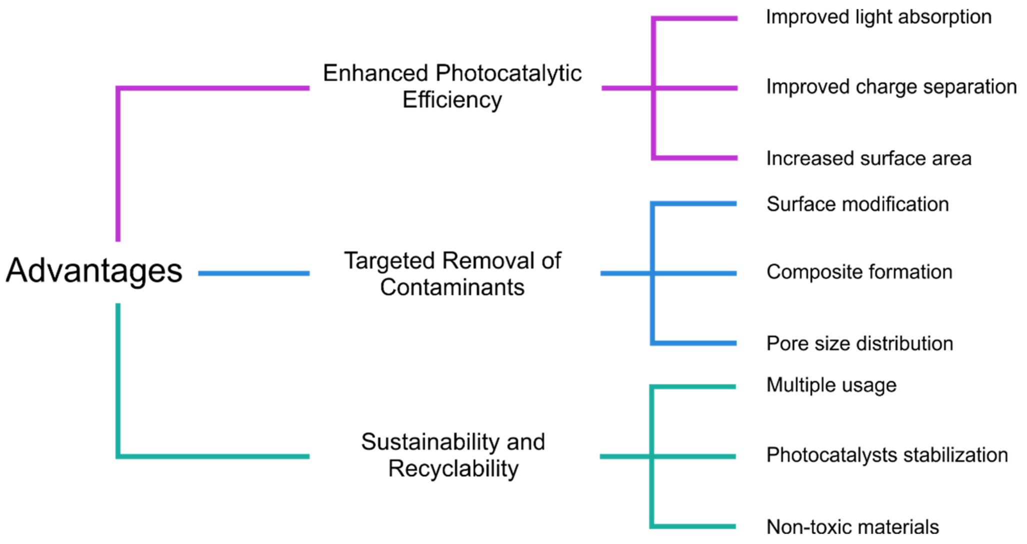

Figure 8. Advantages of polymers in photocatalytic removal of pharmaceutical contaminants from water.

Due to numerous possibilities during synthesis, polymers can be engineered to enhance photocatalytic efficiency through better light absorption and charge separation. For example, the synthesis of photocatalytically active polymers without any additives or metal co-catalysts is one way to enable the forced degradation of contaminants, as demonstrated in a recent paper by Kumar et al. [272]. In this research, the conductive polymer poly(3,4-ethylenedioxythiophene) (PEDOT) was employed for the photocatalytic removal of metformin, a widely utilized molecule with antidiabetic activity that has been found in wastewater due to overuse.

Another essential advantage of polymer application we would like to emphasize is the potential for developing photocatalytic procedures for the forced degradation of contaminants by combining photocatalytic oxide materials with desired photocatalytic properties with polymers. In this way, photocatalytic nanoparticles are incorporated within a polymer medium, creating hybrid composites. This approach brings numerous improvements, one of them being that photocatalytic nanoparticles are tightly immobilized in the polymer medium [273–275], reducing the necessity to filter out nanoparticles later to keep water safe for consumption.

Another advantage essential to showcase is the possibility of functionalizing surfaces with polymers, which allows for targeting specific pharmaceutical pollutants by enhancing the selectivity and effectiveness of the treatment process. For example, in the paper by Park et al. 2013 [276], several polymers were mentioned in the context of modification of TiO_2 surface: polyaniline (PANI), polythiophene, poly(3-hexyl-thiophene) (P3HT), and poly(fluorine-co-thiophene) (PFT). For the TiO_2 photocatalytic materials, according to a series of studies, these polymers have been demonstrated to be able to increase the absorption of visible light and stability [277], charge transfer [278], charge separation [279], and to sensitize the surface in the visible light area [280–282].

Another equally important advantage of polymer applications in the context of photocatalytic removal of pharmaceutical contaminants is related to sustainability and recyclability. Immobilization of photocatalytic nanomaterials within a polymer matrix not only stabilizes the whole system, but also enables multiple uses of the working material. This is crucial because it removes the necessity of filtering out nanoparticles to make the water safe for use. Instead, it is only necessary to remove the entire filter based on the polymer with incorporated photocatalytic nanomaterials [283].

In the context of water purification, it is essential to highlight the non-toxicity of hybrid composites consisting of photocatalytic nanomaterials and polymers. A notable study by Zhao et al. [284] exemplifies this concept by utilizing the well-known PANI to create a novel composite photocatalytic material with $BiVO_4$. This composite not only exhibits superior photocatalytic efficiencies but has also been rigorously tested for toxicity. The material was evaluated against Bacillus subtilis and Staphylococcus aureus, demonstrating non-toxic properties. This finding underscores the potential of such hybrid composites in environmental applications, offering both high efficiency in pollutant degradation and safety for biological systems. The combination of polymers and photocatalytic materials presents a promising approach for developing advanced, eco-friendly photocatalytic materials for effective water purification.

The properties of individual polymers can often be tailored by combination with other materials to achieve a balance of properties that will ensure satisfactory performance under many different conditions. Some applications require a range of mechanical, thermal, electrical, chemical, or optical properties to be achieved in a single product. This diversity of properties is usually achieved by using various additives in the form of discrete particles or fibers. It is generally necessary to modify the surface properties of these particulate or fibrous particles in order to achieve an intimate and enduring association between the additive and the polymer. The large internal surface area available for such associations and the potential increase in macroscopic performance of the filled-polymer systems implies a need for increasing use of heterogeneous oxide fillers. There is also a distinct set of polymers whose degree of crystallinity and mechanical properties are considerably improved with additional phases such as blends or fillers [285,286]. Determining the effect of these different processing techniques, or the properties of the chemically modified phases, on the properties of a heterogeneous polymer often involves the property of interest but also may require extensive measurements such as surface area measurements, surface technique augmentations such as XPS, or the measurement of fundamental packed or porous structures. Characterizing the mechanical properties of these materials is not only of interest from an application perspective, as the most widespread industrial application of polymers is as an engineering material, but it can also tell us more about how the polymers interact at an atomic level [287].

Current challenges include polymer stability, costs, and potential toxicity of degradation products, with one of the greatest being the stability of polymers. Polymers can undergo photo-degradation when exposed to UV or visible light, leading to the breakdown of polymer chains and loss of mechanical and chemical properties. In a recent study by Ran et al. 2018 [288], a well-known conjugated polymer poly(1,3,4-oxadiazole) (POD) was synthesized through readily available synthesis and processing and tested for photocatalytic properties. The authors of the study concluded that although it exhibited excellent photocatalytic properties against selected compounds, its reusability was not ideal because of the relatively poor photostability. However, due to the simplicity of synthesis and processing, further studies and improvements were suggested. In a very interesting study by Chin et al. (2006), different polymeric membranes were tested under conditions typical for photocatalytic degradation, including, among others, the presence of UV light oxidation stress [289]. According to this study, when considering both UV exposure and oxidative test, polytetrafluoroethylene and hydrophobic polyvinylidene fluoride were good choices for photocatalytic applications.

The stability of polymers in water is essential for their use in environmental applications, such as water purification through photocatalysis. Polymers exposed to water, especially under varying pH conditions, can undergo hydrolytic degradation. This involves the breaking of polymer chains due to the reaction with water molecules, which can be accelerated in acidic or alkaline environments. However, in this regard, polymer structures based on polylactic acid (PLA) may offer a solution compared to polymers derived from petroleum [290]. PLA requires much less energy for production compared to petroleum-derived polymers and has the potential to decompose through composting, followed by the release of CO2. On the other hand, PLA has much lower biodegradability, and finding ways to increase the speed of biodegradation was the topic of a recently reported study by Garratt et al. (2023) [291]. In their study, it was demonstrated that the incorporation of

α-Fe_2O_3 into PLA increased the speed of PLA's degradation, resulting in 32% of the solid transforming to the liquid phase, compared to PLA's decomposition alone.

6. Conclusions

In conclusion, this comprehensive review highlights the significant advancements and potential of polymer-based photocatalysts in the removal of pharmaceutical contaminants from water. The unique properties of polymers, including their tunable structures, ease of modification, and ability to enhance the photocatalytic efficiency of other materials, make them promising candidates for sustainable water treatment technologies.

The reviewed literature demonstrates that both organic and inorganic polymers, as well as their hybrids, exhibit excellent photocatalytic properties, enabling efficient degradation of pharmaceuticals. Polyaniline, poly(p-phenylene vinylene), polyethylene oxide, and polypyrrole are among the most studied polymers, showing remarkable results in various photocatalytic applications. The modification techniques, including mechanical blending, extrusion processing, nanocomposite formation, plasma modification, surface functionalization, and cross-linking, play a crucial role in enhancing the photocatalytic activity of polymers.

However, despite the promising results, several challenges remain. The stability of polymers under photocatalytic conditions, the cost of synthesis and modification, and the potential toxicity of degradation products are critical issues that need to be addressed. Future research should focus on developing more robust and cost-effective polymer-based photocatalysts with enhanced stability and reduced environmental impact.

Moreover, the integration of computational methods, such as DFT and TD-DFT, can provide valuable insights into the electronic properties and light absorption characteristics of polymers. This approach can guide the design and optimization of new polymeric materials with superior photocatalytic performance.

Polymer-based photocatalysts offer a promising and sustainable solution for the removal of pharmaceuticals from water. Continued interdisciplinary research, combining experimental and computational approaches, will be essential to overcome existing challenges and fully realize the potential of these materials in environmental protection and water purification.

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