

## Article

# Artificial Neural Network Modeling Enhancing Photocatalytic Performance of Ferroelectric Materials for CO<sub>2</sub> Reduction: Innovations, Applications, and Neural Network Analysis

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## Abstract

Photocatalysis is an emerging technology that harnesses light energy to facilitate chemical reactions. It has garnered considerable attention in the field of catalysis due to its promising applications in environmental remediation and sustainable energy generation. Recently, researchers have been exploring innovative techniques to improve the surface reactivity of ferroelectric materials for catalytic purposes, leveraging their distinct properties to enhance photocatalytic efficiency. With their switchable polarization and improved charge transport capabilities, ferroelectric materials show promise as effective photocatalysts for various reactions, including carbon dioxide (CO<sub>2</sub>) reduction. Through a blend of experimental studies and theoretical modeling, researchers have shown that these materials can effectively convert CO<sub>2</sub> into valuable products, contributing to efforts to reduce greenhouse gas emissions and promote a cleaner environment. An artificial neural network (ANN) was employed to analyze parameter relationships and their impacts in this study, demonstrating its ability to manage training data errors and its applications in fields like speech and image recognition. This research also examined changes in charge separation, light absorption, and surface area related to variations in band gap and polarization, confirming prediction accuracy through linear regression analysis.

**Keywords:** photocatalysis; photocatalytic; ferroelectric material; catalytic; carbon dioxide; artificial neural network; biosensor



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## 1. Introduction

Global climate change refers to the long-term shifts in our planet's weather patterns, impacting temperature, rainfall, and extreme weather events. A major contributor to this change is the rising levels of greenhouse gases in the atmosphere, such as carbon dioxide (CO<sub>2</sub>), methane, and nitrous oxide, which act like a blanket, trapping heat and leading to a warming effect known as the greenhouse effect [1–3]. Carbon dioxide is particularly significant in this context, with much of its increase resulting from our daily activities, especially the burning of fossil fuels for energy, transportation, and industrial processes. Additionally, deforestation and changes in land use release stored carbon back into the atmosphere, further aggravating the situation. This issue affects us all and underscores the urgent need for action to protect our planet [3–5].

The growing buildup of carbon dioxide and other greenhouse gases in our atmosphere is causing the planet to warm, leading to a host of challenges such as rising sea levels, more frequent and intense weather events, disruptions to ecosystems, and threats to our health and well-being. It is essential that we focus on reducing carbon dioxide emissions to combat climate change, and there are several ways to achieve this, including transitioning to cleaner energy sources like renewables, improving energy efficiency, implementing carbon capture and storage technologies, and promoting sustainable land use practices [6–8]. One exciting solution is photocatalysis, a green technology that uses light energy to drive chemical reactions. In the quest to reduce carbon dioxide levels, photocatalysis offers a sustainable method for converting CO<sub>2</sub> into useful products using renewable energy, like sunlight. By harnessing the power of light, photocatalysts can transform CO<sub>2</sub> into fuels or raw materials, helping to lower greenhouse gas emissions and leading us toward a more sustainable future—a hopeful step in our journey to protect the planet for ourselves and future generations [8–11].

Ferroelectric materials contribute to global climate change mainly through their potential applications in clean energy technologies. Ferroelectric materials can change their polarization direction in response to an external electric field. This feature enables efficient charge separation and transfer during photocatalytic reactions, leading to improved catalytic performance and higher rates of conversion of CO<sub>2</sub> to desired products [6]. The unique electronic structure of ferroelectric materials promotes efficient charge transfer on the catalyst surface and facilitates redox reactions involved in CO<sub>2</sub> reduction. This increased charge transfer capability increases the selectivity and efficiency of the photocatalyst and makes it more effective in converting CO<sub>2</sub> into valuable chemicals. Photocatalysis presents several distinct advantages for the reduction of carbon dioxide (CO<sub>2</sub>), making it a critical technology in combating climate change. The incorporation of ferroelectric materials is pivotal due to their ability to generate electric fields under illumination, which enhances the separation of charge carriers and increases the efficiency of CO<sub>2</sub> reduction reactions. Additionally, the switchable polarization of certain photocatalytic materials allows for dynamic control over the catalytic process, enabling optimization for maximum conversion under varying environmental conditions as shown in Figure 1.

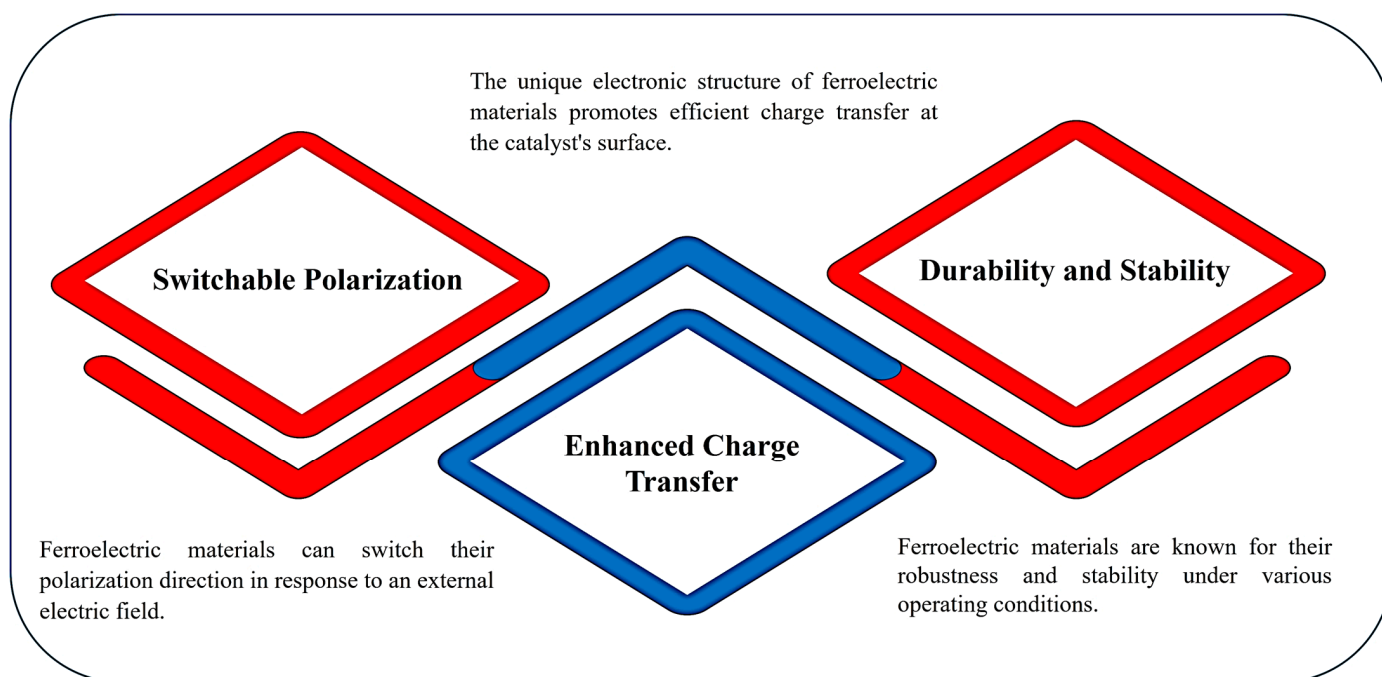


**Figure 1.** Distinct advantages of ferroelectric materials for CO<sub>2</sub>.

Ferroelectric materials are known for their strength and stability in various operating conditions. Their durability ensures long-term performance and reliability in photocatalytic systems, making them suitable candidates for sustainable CO<sub>2</sub> conversion processes [7]. By integrating ferroelectric materials into photocatalytic systems, researchers can develop efficient catalysts to reduce carbon dioxide levels and produce valuable chemicals with minimal environmental impact. This innovative approach has significant potential in addressing the global challenge of climate change and moving towards a more sustainable and greener future. A shallow neural network is a feedforward neural network with one hidden layer. This type of network has been used in this study to investigate and predict the items studied in this study, including charge separation (%), light absorption (%), and surface area (M<sup>2</sup>/G) over a wider range of the band gap (eV) and polarization (μC/CM<sup>2</sup>) as network inputs. Also, with the help of linear regression, the error of the neural network has been evaluated.

## 2. Photocatalytic CO<sub>2</sub> Conversion Optimization

### 2.1. Photocatalysis for Sustainable CO<sub>2</sub> Conversion

In terms of converting carbon dioxide into valuable products, photocatalysis offers a sustainable and environmentally friendly approach to tackling the global challenge of greenhouse gas emissions. Photocatalysis is a process in which a substance known as a photocatalyst uses light energy to accelerate a chemical reaction without consuming the process [8–10]. In this process, the photocatalyst absorbs light (photons) and creates electron–hole pairs, which then participate in redox reactions with other compounds in the surrounding environment. In other words, the key concept of photocatalysis is the use of light energy to activate the photocatalyst, which can facilitate various chemical reactions such as pollutant degradation, water splitting to produce hydrogen, and organic synthesis [11–13]. The ability of photocatalysts to use solar or artificial light to produce chemical transformations makes photocatalysts a potentially sustainable and environmentally friendly technology [14]. The applications of photocatalysts in the decomposition of pollutants in air and water and in the production of renewable energy are given in Table 1. The key principles of photocatalysis and how they can be used to facilitate carbon dioxide conversion are light absorption, charge separation, and surface reactivity.

**Table 1.** Applications of photocatalysis in biosensors.

| Application               | Description                                                                                                                          |
|---------------------------|--------------------------------------------------------------------------------------------------------------------------------------|
| Air Purification          | Photocatalytic systems can decompose volatile organic compounds (VOCs), bacteria, and viruses using TiO <sub>2</sub> under UV light. |
| Water Treatment           | It can break down harmful contaminants into harmless byproducts, making it an essential technology for clean water initiatives.      |
| Hydrogen Production       | Water splitting using photocatalysts can generate hydrogen fuel from water under sunlight.                                           |
| CO <sub>2</sub> Reduction | Converting CO <sub>2</sub> into hydrocarbons or alcohols provides a method for carbon recycling and energy storage.                  |
| Environmental Remediation | Photocatalytic systems can be used for the decomposition of pollutants in air and water.                                             |
| Energy Conversion         | Photocatalysts can be used in the production of renewable energy, such as hydrogen fuel.                                             |

#### 2.1.1. Light Absorption

Photocatalysis relies on the absorption of light by a semiconductor material, usually composed of metal oxides such as titanium dioxide (TiO<sub>2</sub>) or zinc oxide (ZnO). When the

catalyst absorbs photons from sunlight or artificial light sources, it creates electron–hole pairs and creates reactive species that can carry out chemical reactions [15,16]. Indeed, in photocatalysis, the absorption of light by a material creates electron–hole pairs within the material, rather than relying on the material being semi-transparent [17,18]. These photoexcited electron–hole pairs are what drive the catalytic reactions in photocatalysis. The ability of a material to efficiently absorb light and generate these electron–hole pairs is crucial for the success of photocatalysis. The energy of the absorbed photons must be sufficient to promote the electrons to higher energy levels and start the desired chemical reactions. Therefore, while the material used in photocatalysis may not necessarily need to be semi-transparent, it must have suitable light-absorbing properties to efficiently perform electron–hole pair generation and subsequent catalytic reactions [19–21].

### 2.1.2. Load Separation

Excited electrons and positively charged holes created by light absorption in the catalyst material must be effectively separated to prevent recombination. In photocatalysis, when a catalyst material absorbs light energy, it produces excited electrons and positively charged holes. These charge carriers play an important role in redox reactions, such as the reduction of carbon dioxide to produce valuable chemicals such as hydrocarbons [22,23]. However, to effectively utilize these charge carriers and prevent recombination, charge separation is essential. Charge separation refers to efficient partitioning and spatial separation of excited electrons and positively charged holes in the catalyst material. If these charge carriers recombine before participating in the desired reaction, the overall efficiency of the photocatalytic process is significantly reduced [24,25]. Different strategies can be used in photocatalysis to avoid recombination and maximize the utilization of charge carriers. These include designing catalyst materials with suitable band structures to promote charge separation, creating heterogeneous interfaces or junctions within the material to facilitate carrier transfer, and incorporating co-catalysts or sacrificial agents to remove charge carriers and prevent recombination [26]. By optimizing charge separation in photocatalytic systems, increasing the overall efficiency and selectivity of photoinduced charge carrier-induced redox reactions is the goal [12]. It plays a vital role in advancing the development of sustainable energy technologies and processes for converting CO<sub>2</sub> into value-added chemicals in the quest for a greener future.

### 2.1.3. Surface Reactivity

Active sites on the catalyst surface play an important role in facilitating the absorption of reactive molecules such as carbon dioxide and promoting their conversion to the desired products. The surface reactivity of the catalyst can be increased through modifications such as doping with metals or adjusting the crystal structure to improve performance. Surface reactivity plays an important role in the catalysis of chemical reactions, especially in processes such as photocatalysis where catalysts interact with reactant molecules such as carbon dioxide [27,28]. The active sites on the catalyst surface are the key sites where these interactions take place, leading to the adsorption and conversion of molecules into desired products. Increasing the surface reactivity of a catalyst is necessary to improve its performance in certain reactions [29]. One of the common methods used to increase the surface reactivity of the catalyst is through modifications that change its composition or structure [30]. Catalysts can be doped with metals or other elements to introduce additional active sites or to modify the material's electronic properties, thereby increasing its reactivity toward specific molecules [31]. These modifications can create more opportunities for the adsorption and activation of reactants and ultimately promote the desired catalytic transformations. Tuning the crystal structure of a catalyst is another strategy to increase

surface reactivity. By adjusting the arrangement of atoms on the catalyst surface, researchers can optimize the binding energies of reacting molecules and improve the efficiency of catalytic processes. Surface engineering techniques, such as the creation of defects, steps, or specific surface terminations, can also increase the density of active sites and enhance the catalytic activity of materials. Enhancing the surface reactivity of a catalyst through structural modifications and adjustments is a key focus in catalytic research [32]. By tuning the surface properties of catalyst materials, it is possible to design efficient and selective catalysts for various chemical transformations, including the conversion of CO<sub>2</sub> into valuable products, and contribute to the development of sustainable technologies for a greener future. Surface reactivity and active sites are key concepts in understanding the behavior of materials in catalytic reactions, such as carbon dioxide reduction [33]. In the field of materials science, surface reactivity refers to the tendency of a material's surface to interact with other materials, such as reactive molecules, to facilitate chemical reactions [34]. On the other hand, active sites are specific places on the surface of the material where these interactions occur, leading to the initiation and promotion of catalytic reactions. For example, in the case of ferroelectric materials used as photocatalysts for carbon dioxide reduction, the surface reactivity of the material plays an important role in determining its efficiency in converting carbon dioxide into useful products. Active sites on the surface of ferroelectric materials are where interactions between the material and carbon dioxide molecules take place, leading to the activation of carbon dioxide and its transformation into value-added chemicals [35].

## 2.2. Materials and Methods

In this study, we aimed to predict changes in charge separation, light absorption, and surface area across five experimental samples by analyzing their band gap and polarization over a broad range of values. To accomplish this, we employed a feedforward artificial neural network that uses the band gap and polarization as inputs, featuring a hidden layer with five neurons to expedite the process of obtaining accurate results. Our outputs concentrated on charge separation, light absorption, and surface area. We chose a non-linear sigmoid function as the activation function due to its effectiveness in managing the data's complexities, enabling more precise predictions and faster convergence.

During the training of the network, we optimized the error function using the gradient descent algorithm to refine the results. For greater accuracy, we first normalized the input data from our reference table, and after making predictions, we denormalized the results to ensure they fell within an acceptable range. We then compared the fitted graph from our linear regression analysis with a line representing perfect accuracy to evaluate our network's performance. Finally, to assess the accuracy of our predictions, we examined the network's error through linear regression, analyzing the estimated results in normalized form and fitting a graph to visualize these estimates at different points.

The results from our artificial neural network will be explored in detail. In this study, we set out to investigate the potential of ferroelectric materials for sustainable photocatalysis, specifically their role as biosensors to enhance surface reactivity and catalytic efficiency in carbon dioxide reduction. We concentrated on two main input variables: band gap (eV) and polarization ( $\mu\text{C}/\text{cm}^2$ ), and examined three output variables: charge separation (%), light absorption (%), and surface area ( $\text{m}^2/\text{g}$ ). These variables were selected based on a comprehensive review of the existing literature that identified key factors influencing photocatalytic effectiveness. We input these chosen values into an artificial neural network (ANN) model designed to predict and optimize the optimal conditions for improving the photocatalytic properties of these materials. The ANN was configured with appropriate layers and neurons to effectively process the data and generate accurate predictions. Through this methodology,

we aimed to uncover innovative strategies that could significantly enhance the catalytic performance of ferroelectric materials in carbon dioxide reduction applications. A low number of hidden layer neurons can lead to underfitting and high bias, resulting in poor model performance. Too many neurons may cause overfitting, where the model learns noise in the training data and fails to generalize. A hidden layer with five neurons may provide a balanced starting point, but the optimal neuron count varies by problem and dataset.

3. Enhancing Ferroelectric Catalytic Reactivity

In order to increase the surface reactivity of ferroelectric materials for catalytic applications, several strategies can be used. These strategies take advantage of the unique properties of ferroelectric materials, especially switchable polarization and high surface energy [36]. Table 2 shows the key approaches to increase responsiveness. Enhancing the surface reactivity in ferroelectric materials for catalytic applications involves a multifaceted approach that includes applying polarization influence, modifying surfaces with functional groups, using nanostructure techniques, and engineering electrostatic potentials. These strategies not only enhance the catalytic performance, but also open new avenues for research in sustainable energy conversion and environmental remediation.

Table 2. Increasing the surface reactivity of ferroelectric materials for catalytic applications.

|                                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|--------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Utilizing Polarization Effects       | <b>Switchable Polarization</b><br>The inherent polarization in ferroelectric materials can influence surface chemistry. By switching the polarization direction, the adsorption strengths and reaction pathways for reactants can be altered, leading to enhanced catalytic activity. This phenomenon allows selective adsorption of reactants based on the polarization state, effectively overcoming limitations imposed by traditional catalytic principles like Sabatier’s principle. |
|                                      | <b>Band Bending</b><br>The polarization-induced band bending at the ferroelectric/semiconductor interface promotes charge separation and transfer, enhancing photocatalytic performance. This built-in electric field facilitates the separation of photogenerated electrons and holes, increasing their availability for redox reactions.                                                                                                                                                |
| Surface Modification                 | <b>Atomic Dispersion</b><br>Modifying the surface with atoms that bind strongly can increase reactivity. These atoms can remain dispersed on the surface, enhancing catalytic properties without clustering, which often diminishes reactivity.                                                                                                                                                                                                                                           |
|                                      | <b>Functional Group Introduction</b><br>The incorporation of various functional groups (e.g., -OH, -O, -F) on the surfaces of ferroelectric materials like MXenes can modify their electronic properties and enhance their chemical reactivity. This approach tailors the surface for specific reactions by adjusting the electronic environment.                                                                                                                                         |
| Nanostructuring and Thin Films       | <b>Thin Film Technologies</b><br>Utilizing ultrathin ferroelectric films (e.g., less than 3 unit cells thick) allows for easier polarization switching and enhanced surface reactivity due to increased surface-to-volume ratios. This also facilitates better control over the material’s properties and enhances its catalytic performance.                                                                                                                                             |
|                                      | <b>2D Ferroelectric Materials</b><br>Emerging 2D ferroelectric materials exhibit high stability and larger reaction surfaces compared to traditional bulk materials. Their unique properties make them promising candidates for high-efficiency catalysis processes.                                                                                                                                                                                                                      |
| Electrostatic Potential Engineering  | <b>Charge Imbalance Compensation</b><br>The charge imbalance created by polarization can be compensated through electronic reconstruction or atomic rearrangement on the material’s surface. This process can enhance the catalytic efficiency by optimizing the active sites available for reactions.                                                                                                                                                                                    |
| Hybrid Systems with Catalytic Metals | <b>Supported Catalytic Metals</b><br>Integrating ferroelectric materials with metal catalysts can enhance overall reactivity. However, challenges arise from metal clustering; thus, maintaining a well-dispersed state is crucial for effective interaction between the metal and ferroelectric surfaces.                                                                                                                                                                                |

The quest to harness ferroelectric materials for photocatalytic CO<sub>2</sub> reduction has led researchers down a fascinating path of exploration, with a diverse cast of characters including the earthy tones of BiFeO<sub>3</sub> nanoparticles, the sleek, futuristic-looking BaTiO<sub>3</sub> nanosheets, and the versatile PZT nanofibers, each exhibiting unique blends of band gaps ranging from the deep 2.1 eV of BiFeO<sub>3</sub> to the more versatile 3.9 eV of PZT, and the real showstoppers being those materials that can convert CO<sub>2</sub> at rates up to a remarkable 30%, a testament to the transformative power of these ferroelectric champions in the symphony of scientific innovation, all in the pursuit of a greener, more sustainable future (see Table 3).

**Table 3.** Overview of ferroelectric materials for photocatalytic CO<sub>2</sub> reduction [28–34].

| Material                        | Synthesis Method | Morphology | Band Gap (eV) | CO <sub>2</sub> Conversion Rate (%) |
|---------------------------------|------------------|------------|---------------|-------------------------------------|
| BiFeO <sub>3</sub>              | Sol–gel          | NPs        | 2.1           | 20                                  |
| BaTiO <sub>3</sub>              | Hydrothermal     | Nanosheets | 3.2           | 15                                  |
| PZT                             | Solvothermal     | Nanofibers | 3.9           | 25                                  |
| SrTiO <sub>3</sub>              | Co-precipitation | NPs        | 3.2           | 18                                  |
| KNbO <sub>3</sub>               | Solid-state      | Nanosheets | 3.0           | 22                                  |
| PbTiO <sub>3</sub>              | Sol–gel          | Nanofibers | 3.4           | 30                                  |
| Bi <sub>2</sub> WO <sub>6</sub> | Hydrothermal     | Nanosheets | 2.9           | 24                                  |
| LaFeO <sub>3</sub>              | Solvothermal     | NPs        | 2.5           | 21                                  |
| CaTiO <sub>3</sub>              | Co-precipitation | Nanosheets | 3.1           | 19                                  |
| ZnO                             | Solid-state      | Nanofibers | 3.2           | 27                                  |

### 3.1. Surface Engineering

Surface engineering is a crucial approach in the field of photocatalysis for carbon dioxide reduction, as strategically modifying and optimizing the surface properties of catalyst materials can significantly enhance the selectivity and activity of the photocatalytic process. The surface engineering of catalyst materials has a profound impact on their performance in the conversion of carbon dioxide into valuable products using light energy, through various surface modification techniques that can tailor the physical, chemical, and electronic characteristics of the catalyst surface to promote more efficient charge separation, light absorption, and catalytic reactivity. These techniques include controlling the catalyst's surface topography to enhance the accessibility and interaction of reactants; modifying the chemical composition to tune the electronic structure and catalytic properties; attaching functional groups or molecules to alter the wettability, adsorption characteristics, and selectivity; and introducing controlled surface defects to create active sites and influence charge carrier dynamics. The successful integration of these advanced surface engineering strategies into photocatalytic systems holds great promise for the development of highly active and selective catalysts, paving the way for the practical implementation of carbon dioxide utilization technologies and the mitigation of greenhouse gas emissions [29]. Figure 2 shows several surface engineering techniques used in photocatalytic systems for carbon reduction. Techniques such as surface functionalization, in which specific functional groups or metal co-catalysts are introduced onto the surface of a material, can help improve its interactions with reactants and enhance catalytic activity [37]. Surface engineering techniques such as functionalization with specific metal ligands, molecules, or nanoparticles can change the surface chemistry of photocatalysts and create active sites for adsorption, activation, and reaction with carbon dioxide [38,39]. Functional groups can increase the interaction between catalysts and reactants, which leads to improved catalytic activity and selectivity in carbon reduction reactions. By tuning the surface functionalities, it is possible to design catalytic materials with enhanced reactivity and performance for carbon dioxide

conversion [40]. The surface area and porosity of photocatalysts are essential to maximize the exposure of active sites to reactant molecules and light radiation. Surface engineering strategies such as nanostructure, mesopore design, and surface roughness can increase the surface-to-volume ratio of catalyst materials and provide more sites for carbon dioxide adsorption and reaction [37,41]. The increased surface area and porosity promote efficient use of light energy and facilitate rapid transport of reactants and products, improving the overall efficiency of photocatalytic carbon reduction processes. The surface charge and zeta potential of photocatalysts play an important role in the absorption, removal, and migration of charged species involved in carbon dioxide reduction reactions. Surface engineering techniques can be used to tune the surface charge density, distribution of surface functional groups, and electrostatic interactions at the catalyst–liquid interface [42–44].

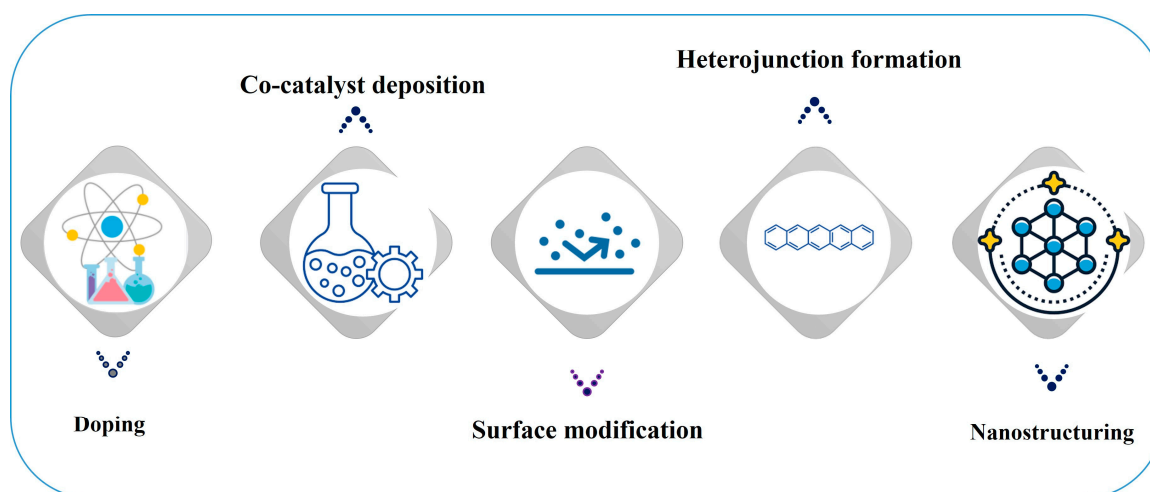


**Figure 2.** Several surface engineering techniques are employed in photocatalytic systems for carbon reduction.

By adjusting the surface charge characteristics, it is possible to influence the adsorption kinetics, surface reactions, and charge transfer processes during photocatalytic carbon reduction and finally optimize the catalytic performance and selectivity of the materials. Surface engineering methods can also use the phenomenon of surface plasmon resonance (SPR) to enhance the light absorption and photoexcitation properties of catalyst materials [45].

By incorporating plasmonic nanoparticles or nanostructures on the surface of photocatalysts, researchers can tune localized electromagnetic fields, increase light harvesting efficiency, and promote the production of hot electrons for catalytic reactions [4]. Exploiting SPR through surface engineering enables precise control over the optical and electronic properties of catalyst surfaces, leading to improved photocatalytic performance in carbon reduction processes [46]. Also, surface engineering approaches can address the stability and corrosion challenges that photocatalysts face during long-term operation in carbon reduction reactions. By covering catalyst surfaces with protective layers, deactivating active sites, or modifying surface compositions, the resistance of materials to photo corrosion, chemical degradation, and surface poisoning can be increased. Improved stability and corrosion resistance through surface engineering ensure the long-term performance and durability of photocatalysts in carbon dioxide conversion applications [35,47].

### 3.2. Defect Engineering

Manipulating the presence of defects on the material surface can create additional active sites for catalytic reactions. By controlling the type and density of defects, the catalytic performance of the material increases. Defect engineering in the field of photocatalysis

for carbon dioxide reduction involves the deliberate manipulation of defects in catalyst materials to enhance their performance in converting carbon dioxide into value-added products such as fuels and chemicals [48,49]. Defects in photocatalysts can create localized states in the band structure that facilitate charge separation and migration [50]. These defects can act as trapping sites for charge carriers, increasing their lifetime and promoting efficient utilization in catalytic reactions. By adjusting the type and density of defects, the charge separation efficiency of photocatalysts is increased, which leads to the improvement of carbon dioxide conversion. In active site engineering, defects in catalyst materials can serve as active sites for the absorption, activation, and conversion of reactants involved in the carbon dioxide reduction process. Surface defects, vacancies, and impurities can change the electronic and chemical properties of catalysts and affect the binding energies of intermediates and reaction kinetics [51,52]. Through defect engineering, researchers can tune the accessibility and reactivity of active sites, thereby optimizing catalytic activity and selectivity for carbon dioxide conversion. Defects in photocatalysts can cause changes in the band structure, band gap, and energy levels, affecting photon absorption and electron–hole pair generation during light excitation. By strategically introducing defects, one can change the position of the energy levels, improve the light-harvesting efficiency, and promote the production of reactive radicals to reduce carbon dioxide. Controlling the band structure through defect engineering enables precise control of the photocatalytic performance of materials. Defect engineering can also play an important role in increasing the stability and durability of photocatalysts under harsh reaction conditions [53,54]. By stabilizing defects, deactivating surface sites, and preventing defect-induced degradation pathways, researchers can develop robust catalytic materials capable of sustained catalytic activity over long-term reaction cycles. The design of defect-resistant catalysts is essential for long-term performance and practical application in carbon dioxide reduction processes. In some cases, the synergistic interaction of defects with other agents, such as co-catalysts, dopants, or supports, can enhance the overall performance of photocatalytic systems for carbon dioxide reduction. By carefully designing composite materials that take advantage of the complementary effects of defects and other components, researchers can achieve synergistic improvements in catalytic activity, selectivity, and stability, and enhance the efficiency of carbon dioxide conversion technologies [55].

### 3.3. Surface Optimization Strategies

Increasing the surface area of the material through nanostructure or creating a porous architecture can expose more active sites for catalytic reactions and thus improve the efficiency of the material as a catalyst. Surface optimization is a critical aspect in the design and development of photocatalysts for carbon reduction reactions. Maximizing the surface area of catalyst materials increases their efficiency in absorbing light energy, promoting catalytic reactions, and improving the overall performance of photocatalytic systems [56]. In order to optimize the surface in the field of photocatalysis for carbon reduction, there are several key strategies, as shown in Figure 3. The use of nanostructured materials such as nanoparticles, nanowires, nanosheets, or nanotubes can significantly increase the level of photocatalysts. The high surface-to-volume ratio of nanostructures provides many active sites for carbon dioxide absorption and reaction and increases the efficiency of photocatalytic processes. By engineering the size, shape, and morphology of the nanostructures, researchers can tune the surface area and expose more reactive sites for efficient carbon reduction reactions under light irradiation [57,58]. The incorporation of mesoporous structures in photocatalysts allows the creation of interconnected pore networks with well-defined pore size and distribution. Mesoporous materials offer a large internal surface area accessible to reactant molecules, enabling efficient diffusion of carbon dioxide and products into the

catalyst matrix. By controlling the porosity and pore architecture of materials, researchers can optimize the available surface area for catalytic interactions and enhance mass transfer and reaction kinetics in photocatalytic carbon reduction processes [59]. The introduction of surface roughness or texture on the catalyst material can further increase the effective surface available for catalytic reactions. Rough surfaces create additional active sites, defects, and surface steps that facilitate the adsorption and activation of carbon dioxide molecules. Surface roughness enhances the light scattering and trapping properties of photocatalysts, increases light harvesting efficiency, and enhances photon-to-electron conversion for carbon reduction reactions [60]. By adjusting the surface morphology and roughness, researchers can maximize the surface area and light utilization of the materials and improve their photocatalytic performance [61]. The design of hierarchical architectures composed of multiple length scales, such as micro-/meso-/nano-features, provides a synergistic approach for surface optimization in photocatalytic systems. Hierarchical structures combine the advantages of different-length scales, and provide a high surface area, enhanced light absorption, and efficient charge separation pathways for photocatalytic carbon reduction. By integrating hierarchical architectures into catalyst materials, researchers can take advantage of multiscale surface morphologies to achieve superior catalytic activity, stability, and selectivity under light-driven conditions [62]. Applying thin coatings, surface modifications, or functional groups on catalyst surfaces can also improve the surface area for catalytic reactions. Coatings can prevent aggregation, passivate surface defects, and increase access to active sites for carbon dioxide adsorption and activation. Functional groups can introduce specific binding sites, facilitate surface electron transfer processes, and modulate the surface chemistry of photocatalysts, leading to increased catalytic performance in carbon reduction reactions [63]. By tuning the surface properties through coating and functionalization, researchers can optimize the surface and reactivity of materials for efficient photocatalysis. Optimizing the surface of photocatalysts is necessary to maximize their catalytic efficiency and performance in carbon reduction reactions. Using nanostructures, mesopore design, surface roughness, hierarchical architectures, and surface coating strategies, researchers can increase the surface area available for catalytic interactions, improve light harvesting efficiency, and convert carbon dioxide into products with value under light radiation [64]. Surface optimization is important in advancing the development of sustainable energy technologies based on photocatalytic processes for carbon reduction and environmental remediation programs [65].

### 3.4. Adjusting the Electronic Structure

Modifying the electronic structure of the material by doping or alloying can change its surface properties and increase its reactivity towards specific reactants. Tuning the electronic structure in the field of photocatalysis for carbon dioxide reduction involves manipulating the electronic properties of catalyst materials to enhance their performance in converting carbon dioxide into valuable products using light energy [66,67]. Various strategies can be employed to tune the electronic structure of photocatalysts for carbon dioxide reduction. Introducing impurity atoms into the catalyst material can change its electronic structure by changing the number of charge carriers or changing the position of energy levels [68]. It can improve the catalytic activity and selectivity of materials. Alloying, by mixing different metals to form alloys, can create synergistic effects that increase the catalytic performance of materials. Alloying can also lead to changes in the electronic structure, such as tuning the band gap or improving charge separation [68,69]. Tuning the photocatalyst band gap through structural changes or chemical treatment can enable the absorption of a wider range of light wavelengths and improve the efficiency of the carbon dioxide reduction reaction. Therefore, understanding the surface reactivity and active sites

is essential for the design and optimization of materials for catalytic applications [70,71]. By tuning these properties, efficient catalysts can be made for a wide range of reactions, including carbon dioxide reduction, with potential implications for sustainable energy production and environmental remediation efforts.

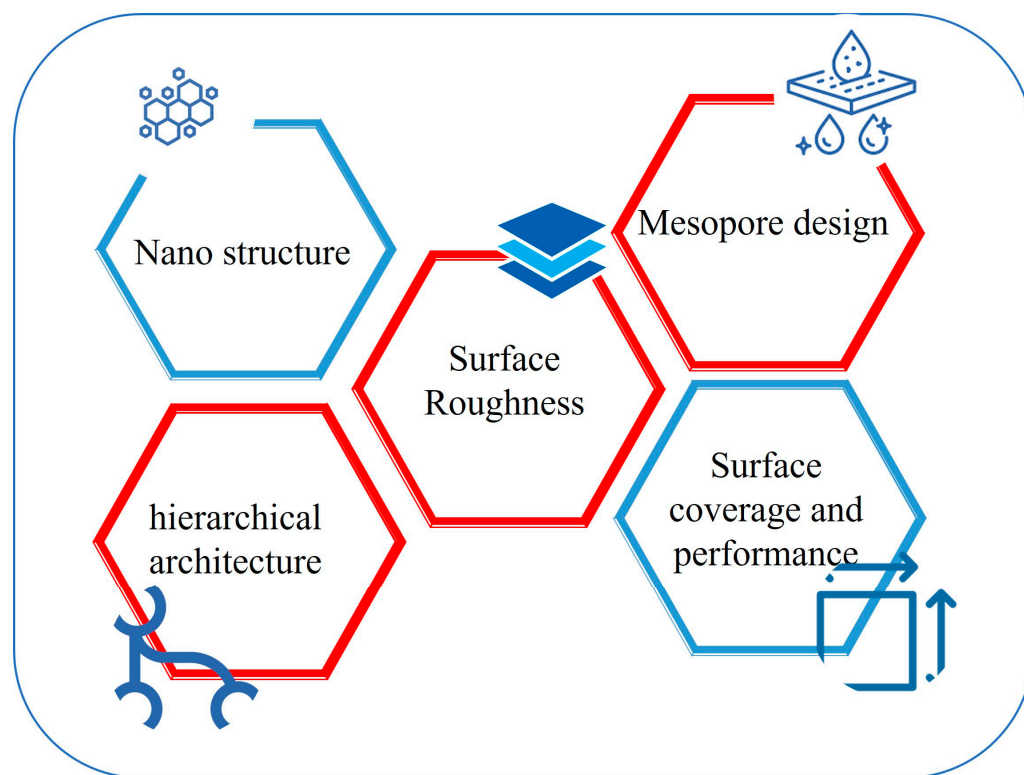


**Figure 3.** Key strategy for surface optimization in the field of photocatalysis for carbon reduction.

#### 4. Advantage of Ferroelectric Materials as Photocatalysts

This unique property of ferroelectrics can be used for photocatalytic applications due to their ability to increase charge separation and improve overall efficiency in catalytic reactions, such as carbon dioxide reduction [72]. When ferroelectrics are used as photocatalysts, the intrinsic electrical polarization facilitates the spatial separation of photo charge carriers (electrons and holes) upon exposure to light [73]. This is because the internal electric field in ferroelectric materials can act as a driving force to separate charges and prevent their recombination, which is a common loss mechanism in many photocatalytic processes. The surface of a ferroelectric photocatalyst can act as a potential well for light-excited electrons and holes, helping to trap them near the surface and increase their lifetime. The separated charges can participate more effectively in redox reactions, leading to improved catalytic performance [74]. In addition, the unique electronic structure of ferroelectric materials can facilitate fast charge transfer processes between the catalyst and reactants and promote the production of reactive intermediates necessary for the desired chemical transformations [75].

##### 4.1. Electrical Properties

Ferroelectric materials often have unique electrical properties that allow the transport of electrons and holes. These electrical properties are among the properties that introduce ferroelectric compounds as powerful photocatalysts [67]. Ferroelectric materials, including barium strontium titanate ( $\text{BaSrTiO}_3$ ), exhibit unique electrical properties that make them particularly suitable for photocatalytic applications, particularly in  $\text{CO}_2$  reduction [58,76]. This feature enables controlled manipulation of the material's electrical state, which can

enhance charge separation and reduce recombination rates during photocatalytic processes. Ferroelectric materials typically have a high dielectric constant, which allows them to store and release electrical energy efficiently. This feature is useful in photocatalytic applications, as it helps maintain a stable electric field that can facilitate the separation of charge carriers generated during light absorption [77,78]. All ferroelectric materials are inherently piezoelectric and pyroelectric. This means they can generate an electrical charge in response to mechanical stress (piezoelectric) or temperature changes (pyroelectric). These effects can be used to enhance photocatalytic activity by improving charge carrier dynamics and overall efficiency [53,79].

#### 4.2. Optical Properties

Ferroelectric materials usually have special optical properties that enable the absorption of light and the creation of electron–hole pairs. These features are very important because light can provide the necessary energy to start the photocatalytic process. Ferroelectric materials have unique optical properties that enable light absorption and generation of electron–hole pairs, which are critical for the initiation of photocatalytic processes [80]. Ferroelectric materials exhibit a strong interaction with light, allowing them to absorb photons efficiently. This interaction is very important for creating electron–hole pairs when the material is turned on. The ability to absorb light at different wavelengths, especially in the UV and visible regions, increases their photocatalytic activity. The band gap of ferroelectric materials can be engineered through doping or compositional modifications, enabling them to respond to visible light. For example, modifications can narrow the band gap, allowing these materials to utilize a wider range of sunlight for photocatalytic applications [81]. This is particularly important for increasing the efficiency of CO<sub>2</sub> reduction processes. Spontaneous polarization in ferroelectric materials contributes to their photovoltaic behavior, where absorbed light produces charge carriers that can be efficiently separated due to the internal electric field created by the polarization. This separation minimizes recombination losses and leads to improved photocatalytic efficiency [82]. Photoexcitation of ferroelectric materials can lead to phenomena such as photo contraction and changes in polarization states, which further increase the charge carrier dynamics. These effects facilitate more efficient pathways for chemical reactions during photocatalysis [83].

#### 4.3. Sustainability

Ferroelectric materials can have good chemical and thermal stability, which allows continuous use in photocatalytic processes. The stability of these materials is very important in improving the efficiency and useful life of photocatalysts. Ferroelectric materials are characterized by their unique electrical and optical properties, which significantly contribute to their chemical and thermal stability [51]. These features are very important for increasing the efficiency and lifetime of photocatalysts used in CO<sub>2</sub> reduction processes. Ferroelectric materials usually exhibit good chemical stability, which allows them to withstand the harsh environmental conditions often encountered during photocatalytic reactions [84]. This minimizes degradation resistance over time and ensures that the material maintains its structural integrity and performance. The stability of ferroelectric materials also affects their interaction with reactants [52,85]. A stable material can effectively promote surface reactions without undergoing significant changes that could hinder catalytic activity. This is especially important when dealing with species active in reducing CO<sub>2</sub>. Many ferroelectric materials have a high Curie temperature, above which they change from the ferroelectric state to the paraelectric state. This property is beneficial for photocatalysis because it allows the material to operate efficiently at high temperatures without losing its ferroelectric properties. Thermal stability ensures that ferroelectric materials can operate effectively over

a wide range of temperatures, which is critical for real-world applications where conditions may fluctuate. This compatibility can lead to improved photocatalytic performance in different operating environments [67,86].

## 5. Ferroelectric Material as a Photocatalyst to Reduce Carbon Dioxide

Several ferroelectric materials have been identified as effective photocatalysts for CO<sub>2</sub> reduction. These materials use their unique ferroelectric properties to improve the efficiency of photocatalytic processes, making them valuable candidates for addressing environmental challenges associated with CO<sub>2</sub> emissions. Figure 4 shows some of these materials.

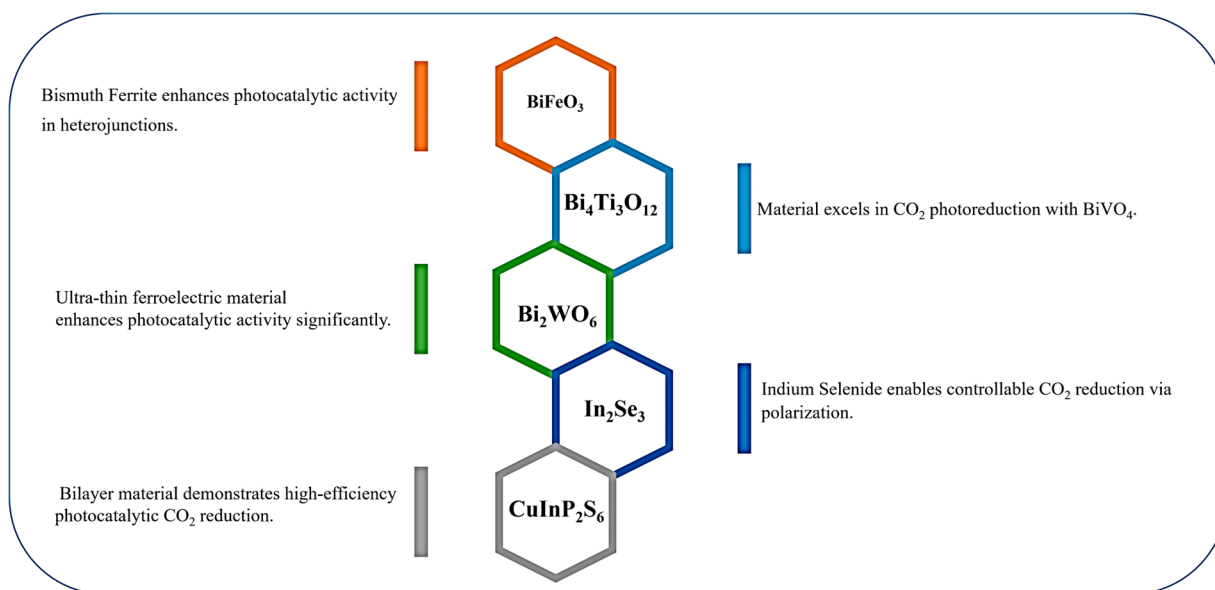


**Figure 4.** Ferroelectric materials used as photocatalysts.

### 5.1. Bismuth Ferrite ( $\text{BiFeO}_3$ )

The bismuth-iron-oxide ferroelectric material shines as a remarkable photocatalyst, captivating researchers with its ability to efficiently convert carbon dioxide into valuable fuels like methane and methanol under visible light. Its spontaneous electric polarization, which can be manipulated, enables exceptional charge separation and transport, boosting the overall photocatalytic efficiency. Researchers are determined to further optimize the material's composition and unravel the underlying mechanisms, recognizing the immense potential of this ferroelectric catalyst in developing sustainable energy technologies and addressing the global challenge of climate change [87].  $\text{BiFeO}_3$  shows ferroelectric properties due to its unique crystal structure, which allows spontaneous polarization. Its optical band gap is approximately 2.2 eV; this enables it to efficiently absorb visible light, which is crucial for photocatalytic applications. This band gap allows  $\text{BiFeO}_3$  to generate electron-hole pairs when exposed to visible light, facilitating various photocatalytic reactions [88,89]. These charge carriers can participate in redox reactions that degrade organic pollutants. Research has shown that doping  $\text{BiFeO}_3$  with various elements, such as gadolinium (Gd) or manganese (Mn), can significantly increase its photocatalytic efficiency. Gd doping to improve carrier separation and decrease recombination rates leads to increased photocatalytic activity. Similarly, the introduction of bismuth into the structure modifies the lattice parameters and reduces the band gap, further enhancing the photocatalytic performance. Different synthesis methods affect the morphology and crystallinity of  $\text{BiFeO}_3$  nanoparticles, which in turn affects their photocatalytic efficiency. Techniques such as

sol–gel synthesis and auto-ignition have been used to produce nanoparticles with optimal sizes and surface areas that maximize light absorption and catalytic activity [90–92].

### 5.2. Barium Titanate

BaTiO<sub>3</sub> is another ferroelectric material that has been investigated for its photocatalytic properties. It shows good stability and efficiency in converting CO<sub>2</sub> to fuel using solar energy. Barium titanate (BaTiO<sub>3</sub>) is a widely studied ferroelectric material that is notable for its potential as a photocatalyst, particularly in the reduction of CO<sub>2</sub> [93]. Its unique properties and structural features make it suitable for various photocatalytic applications. Barium titanate has a perovskite structure that contributes to its ferroelectric properties [94]. The band gap of BaTiO<sub>3</sub> is typically around 3.2 eV, which allows it to effectively absorb UV light. However, the modifications can increase its visible light absorption capability, which is very important for photocatalytic activity. Recent advances in nanoscale synthesis of BaTiO<sub>3</sub> have led to materials with controlled morphology and properties. Techniques such as sol–gel synthesis and hydrothermal methods enable the production of nanoparticles, nanowires, and other forms that increase the surface area and reactivity of BaTiO<sub>3</sub> for photocatalytic applications [95,96].

### 5.3. Lead Zirconate Titanate (Pb(Zr,Ti)O<sub>3</sub> or PZT)

Lead zirconate titanate (Pb(Zr,Ti)O<sub>3</sub>), commonly known as PZT, is a remarkable ferroelectric material that has attracted attention for its photocatalytic properties, particularly in the reduction of CO<sub>2</sub>. Its unique properties make it a valuable candidate in the field of photocatalysis. PZT exhibits strong ferroelectric behavior due to its perovskite structure. This structure allows for spontaneous polarization that can be manipulated through external electric fields. Ferroelectric properties enhance charge separation and mobility, which are very important for photocatalytic applications [97]. The band gap of PZT typically ranges from 3.0 to 3.5 eV, which makes it primarily responsive to UV light. However, modifications such as doping with other elements can reduce the band gap and allow better absorption of visible light. This is necessary to improve the efficiency of solar photocatalytic processes [98,99].

### 5.4. Strontium Titanate (SrTiO<sub>3</sub>)

Strontium titanate (SrTiO<sub>3</sub>) is a promising ferroelectric material that has attracted attention due to its potential as a photocatalyst in CO<sub>2</sub> reduction. Its unique properties and mechanisms make it an effective candidate for converting CO<sub>2</sub> into renewable fuels [100–102]. SrTiO<sub>3</sub> has a perovskite structure, which is essential for its ferroelectric behavior. This structure enables spontaneous polarization, increased charge separation, and mobility, which are critical for photocatalytic processes. The band gap of SrTiO<sub>3</sub> is about 3.2 eV, which primarily responds to UV light. However, modifications such as doping with transition metals can reduce the band gap and cause better absorption of visible light, thereby improving its photocatalytic efficiency [64,103]. Furthermore, alternative doping strategies can lower the energy barriers for intermediate formation and further optimize the reduction process [58,104].

### 5.5. Barium Strontium Titanate (Ba,Sr)TiO<sub>3</sub>

This solid solution of ferroelectric materials has attracted attention due to its photocatalytic activity in CO<sub>2</sub> reduction. The composition can be optimized to increase the photocatalytic performance of the material for CO<sub>2</sub> conversion. Barium strontium titanate is a remarkable ferroelectric material that has emerged as a promising photocatalyst for CO<sub>2</sub> reduction. Its unique structural and electronic properties make it particularly effective in this application. Barium strontium titanate combines the properties of barium titanate

(BaTiO<sub>3</sub>) and strontium titanate (SrTiO<sub>3</sub>), resulting in a perovskite structure that exhibits strong ferroelectric behavior [104]. This structure allows high polarization and enhances charge separation, which is very important for photocatalytic processes. The band gap of BaSrTiO<sub>3</sub> can be tuned through the ratio of barium to strontium, which generally ranges from 3.0 to 3.5 eV [105]. This tunability increases visible light absorption when doped or modified and is more effective for photocatalytic applications compared to traditional semiconductors. Doping BaSrTiO<sub>3</sub> with transition metals or creating a composite with other materials can significantly improve its photocatalytic performance. For example, doping with elements such as nickel or cobalt can increase light absorption and improve charge carrier dynamics [106,107]. Ferroelectric materials exhibit unique properties that can significantly increase the photocatalytic and electrocatalytic reduction of CO<sub>2</sub> to valuable compounds such as methane and formic acid. The mechanisms by which these substances facilitate CO<sub>2</sub> reduction involve several key factors. Four of the specific mechanisms that strengthen ferroelectric materials are given in Figure 5. Ferroelectric materials have spontaneous polarization that creates an internal electric field, which increases charge separation [86,108]. This polarization can direct electrons and holes to different regions within the material, thereby reducing the probability of recombination and increasing the availability of charge carriers for chemical reactions. For example, in ferroelectric Bi<sub>3</sub>TiNbO<sub>3</sub> nanosheets, enhanced polarization was shown to facilitate bulk charge separation, improving photocatalytic performance for CO<sub>2</sub> reduction [70,77]. The direction of polarization in ferroelectric materials can affect the adsorption properties of reactants on their surfaces. Different polarization states can lead to changes in the electronic structure on the surface that allow selective adsorption of CO<sub>2</sub> molecules. This ability to control surface interactions helps to optimize reaction pathways and product selection during CO<sub>2</sub> conversion processes. Introducing oxygen vacancies (OVs) to ferroelectric materials can increase their catalytic properties [94,109]. OVs not only improve light absorption, but also facilitate the adsorption and activation of CO<sub>2</sub> molecules on the catalyst surface. For example, studies have shown that combining ferroelectric polarization with OVs in materials such as Bi<sub>3</sub>TiNbO<sub>3</sub> results in effective photocatalytic CO<sub>2</sub> reduction by broadening photo absorption and stabilizing charge carriers [110]. In electrocatalytic applications, ferroelectric materials can be engineered to change their polarization state, which allows for dynamic control over reaction pathways and product formation. Transition metals anchored on ferroelectric substrates such as  $\alpha$ -In<sub>2</sub>Se<sub>3</sub> can modulate their catalytic performance through ferroelectric switching and affect the d-band center and thus the reactivity towards CO<sub>2</sub>. This capability enables precise setting of limiting potentials and selectivity of desired products such as methane or formic acid. Fabrication of heterogeneous junctions between ferroelectric materials and other semiconductors can create synergistic effects that increase photocatalytic efficiency. These heterogeneous junctions can provide better charge transfer and improved light absorption properties and further reduce CO<sub>2</sub> to useful compounds [111,112].

Innovative research in covalent organic frameworks, nanocomposites, and perovskite catalysis is advancing CO<sub>2</sub> photocatalysis and carbon capture. Comprehensive reviews, novel material synthesis, and fundamental simulations demonstrate the versatility of these approaches in enhancing light absorption, charge separation, and sustainable chemical production to address climate change [112–116]. The integration of these strategies holds immense promise for transformative solutions towards a sustainable future.

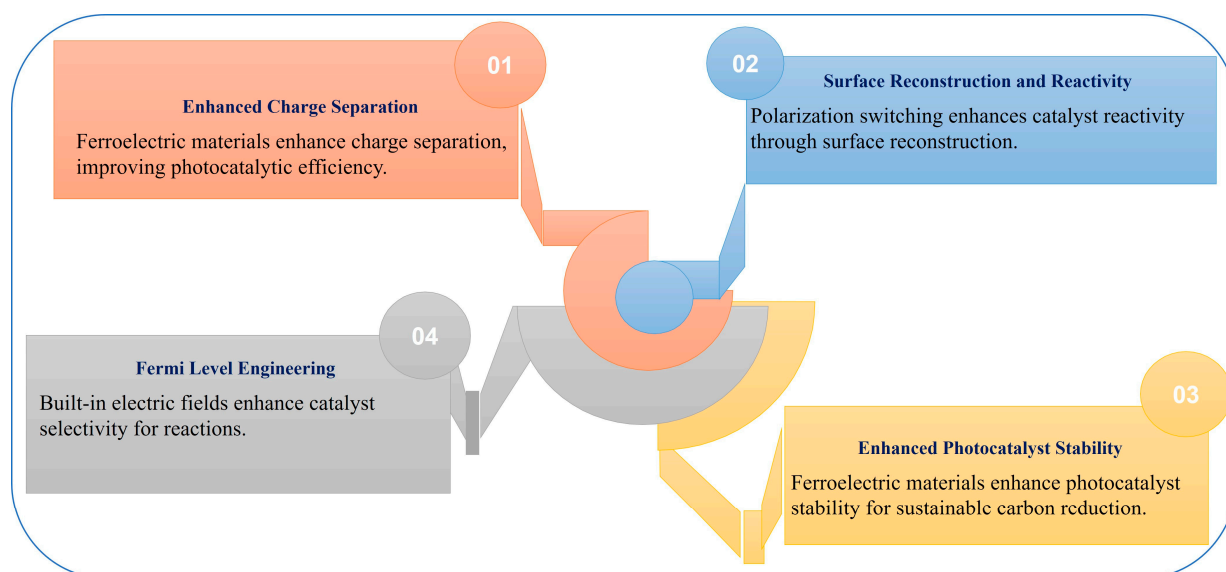


**Figure 5.** Four cases of special mechanisms that strengthen ferroelectric materials.

## 6. Results and Discussion

To predict how charge separation (%), light absorption (%), and surface area ( $\text{M}^2/\text{G}$ ) change with increasing band gap (eV) and polarization ( $\mu\text{C}/\text{cm}^2$ ), we created a feedforward neural network based on the data in Table 4. This network helps us understand how these properties vary within a band gap range of 0 to 3.4 eV and polarization levels from 0 to 90  $\mu\text{C}/\text{cm}^2$ . In Figure 6, you can see a schematic of the artificial neural network, which features a hidden layer of five neurons. The neural network model presented in this work takes two key material properties as inputs—the band gap energy (in eV) and the polarization (in  $\mu\text{C}/\text{cm}^2$ )—across a dataset of eight different samples. Using this input data, the model is trained to predict the corresponding values for three important performance metrics: charge separation efficiency, light absorption capability, and specific surface area.

Figure 7 shows the predicted results from the neural network model regarding the changes in charge separation efficiency, with the key observations indicating that as the material's band gap energy increases, the percentage of photogenerated charge carriers that undergo successful separation initially remains relatively constant; however, beyond a band gap of approximately 2 eV, the charge separation efficiency exhibits a sharp decline, before subsequently increasing again. Interestingly, the data suggest that variations in the material's polarization do not result in any significant changes in the charge separation efficiency, implying that the band gap energy is the dominant factor influencing the charge separation process within the studied system, at least within the range of polarization values considered. This provides valuable insights into the fundamental charge transport mechanisms governing the photocatalytic performance of the materials under investigation, and the neural network model's ability to accurately predict the changes in charge separation efficiency as a function of the material properties. In turn, this showcases the power of data-driven approaches in uncovering the underlying structure–property relationships to guide the rational design of novel photocatalytic materials with enhanced charge separation and improved catalytic activity for the desired transformation of  $\text{CO}_2$ , which is a key consideration in the design of effective photocatalysts for applications such as  $\text{CO}_2$  reduction.

**Table 4.** Photocatalytic efficiency of ferroelectric materials for carbon dioxide reduction using a nanotech sensor.

| Material                                               | Synthesis Method | Morphology    | Band Gap (eV) | Polarization (μC/cm <sup>2</sup> ) | Charge Separation (%) | Light Absorption (%) | Surface Area (m <sup>2</sup> /g) | CO <sub>2</sub> Conversion Rate (μmol/g·h) | Product Selectivity (%) | Stability (h) | Sensor Integration (%) |
|--------------------------------------------------------|------------------|---------------|---------------|------------------------------------|-----------------------|----------------------|----------------------------------|--------------------------------------------|-------------------------|---------------|------------------------|
| BiFeO <sub>3</sub>                                     | Sol-gel          | Nanoparticles | 2.2           | 90                                 | 75                    | 80                   | 85                               | 120                                        | 85 (CH <sub>4</sub> )   | 100           | 92                     |
| BaTiO <sub>3</sub>                                     | Hydrothermal     | Nanofibers    | 3.2           | 26                                 | 65                    | 70                   | 95                               | 90                                         | 75 (HCOOH)              | 80            | 88                     |
| Pb(Zr,Ti)O <sub>3</sub>                                | Solvothermal     | Nanosheets    | 3.4           | 35                                 | 72                    | 75                   | 90                               | 110                                        | 80 (CH <sub>4</sub> )   | 90            | 90                     |
| SrTiO <sub>3</sub>                                     | Solid-state      | Nanocubes     | 3.2           | 18                                 | 68                    | 65                   | 80                               | 85                                         | 72 (HCOOH)              | 70            | 85                     |
| (Ba,Sr)TiO <sub>3</sub>                                | Co-precipitation | Nanoparticles | 3.0           | 30                                 | 70                    | 75                   | 92                               | 100                                        | 82 (CH <sub>4</sub> )   | 85            | 92                     |
| Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub>        | Molten-salt      | Nanosheets    | 2.9           | 40                                 | 75                    | 80                   | 88                               | 115                                        | 78 (HCOOH)              | 95            | 88                     |
| KNbO <sub>3</sub>                                      | Hydrothermal     | Nanofibers    | 3.1           | 22                                 | 62                    | 68                   | 90                               | 80                                         | 70 (CH <sub>4</sub> )   | 75            | 85                     |
| Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub> | Sol-gel          | Nanoparticles | 3.0           | 38                                 | 68                    | 72                   | 85                               | 95                                         | 75 (HCOOH)              | 80            | 90                     |

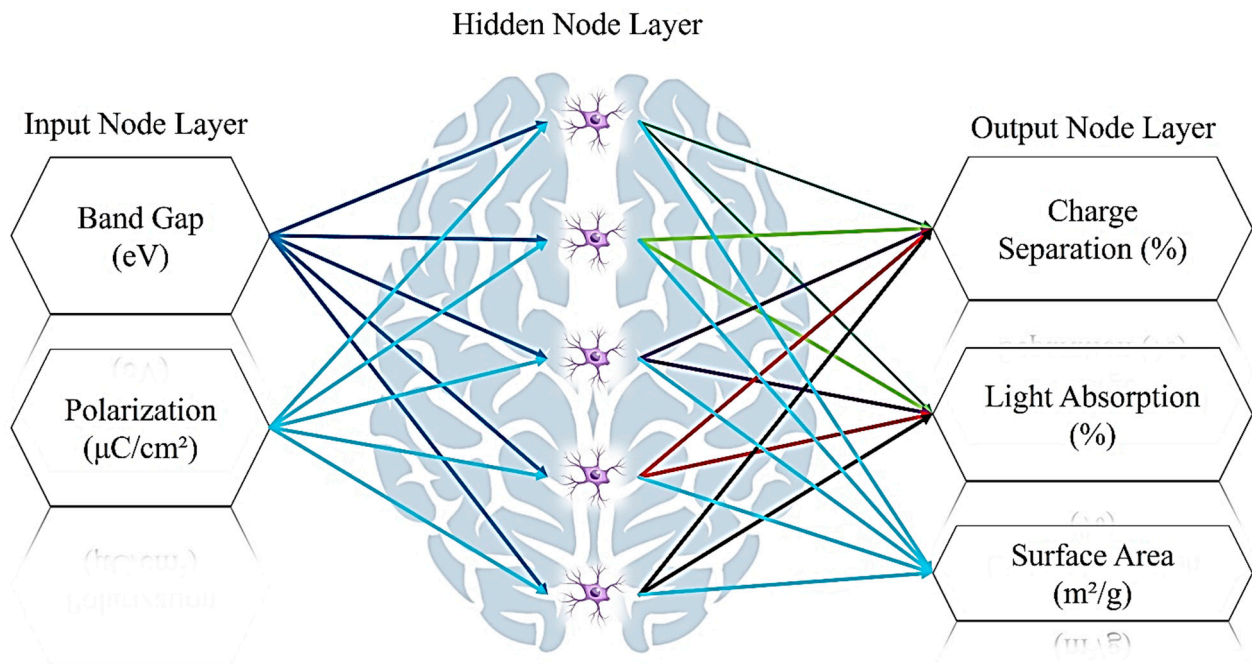


**Figure 6.** Schematic of an ANN with a hidden layer for photocatalytic efficiency of ferroelectric materials for carbon dioxide reduction using a nanotechnology sensor.

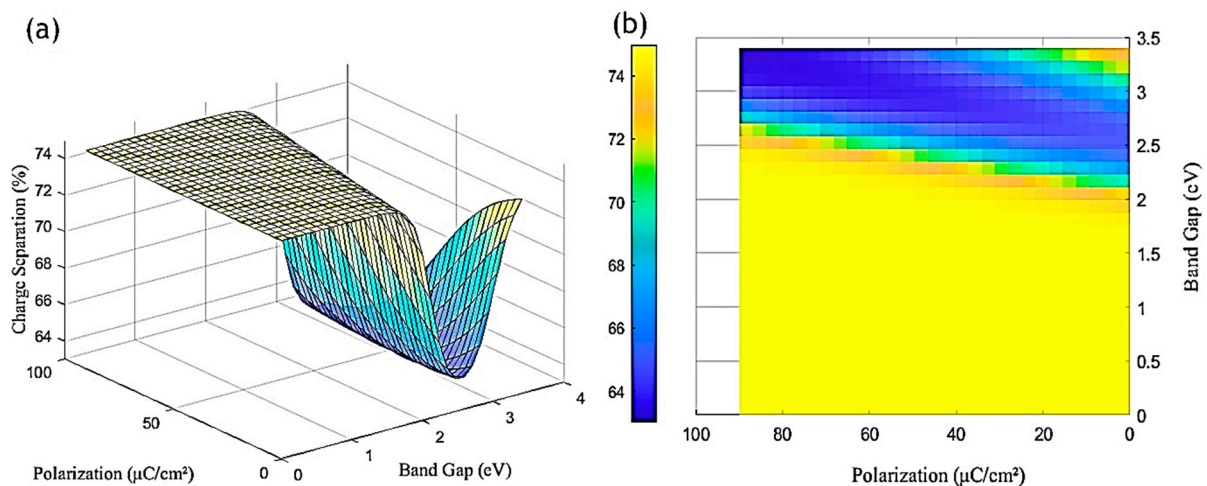


**Figure 7.** Predictions made by the artificial neural network of the charge separation of the test object in this study: (a) front view and (b) side view.

Figure 8 shows the predictions made by the neural network regarding changes in light absorption. From these results, we can see that as the band gap increases, light absorption tends to decrease. On the other hand, when polarization levels rise, light absorption increases. Figure 9 presents the network's predictions for changes in surface area. It indicates that surface area decreases as the band gap increases, while higher polarization leads to a sharp drop in surface area, which then levels off after a certain point. Finally, Figure 10 shows the results from the linear regression analysis related to our inputs and outputs. As expected, the artificial neural network was able to predict charge separation (%), light absorption (%), and surface area ( $M^2/G$ ) with remarkable accuracy, showing an error rate of less than 1% compared to the target values listed in Table 4. Photocatalytic  $CO_2$  reduction involves the use of light to convert carbon dioxide into valuable chemicals or fuels. The process is energy efficient and environmentally friendly, offering a potential solution to global warming and energy crises. Ferroelectric materials are characterized by

switchable polarization, which can significantly affect the physical and chemical properties of the surface. These materials are attractive candidates for photocatalysts due to their unique properties. Nanotechnology plays an important role in enhancing the efficiency of photocatalytic processes. Nanoscale sensors can monitor and optimize the conditions for CO<sub>2</sub> reduction, ensuring higher efficiency and better control over the reaction [2]. Recent studies [4–11] have focused on the composition and properties of ferroelectric materials and their potential as photocatalysts. Researchers have investigated various preparation methods such as ion doping, thermal treatment, and plasma etching to enhance the photocatalytic performance of these materials [3]. While significant progress has been made, challenges remain, such as the stability of ferroelectric materials and the need for advanced characterization techniques. Future research will aim to develop more efficient and stable photocatalysts, potentially revolutionizing CO<sub>2</sub> reduction technologies [3]. Figure 10 shows the pivotal impact of surface engineering on improving the photocatalytic performance for CO<sub>2</sub> reduction. The data showcase the substantial benefits of the surface engineering approach, with the surface-engineered catalyst demonstrating a significantly higher selectivity towards valuable reduction products like methane and methanol compared to the pristine catalyst.

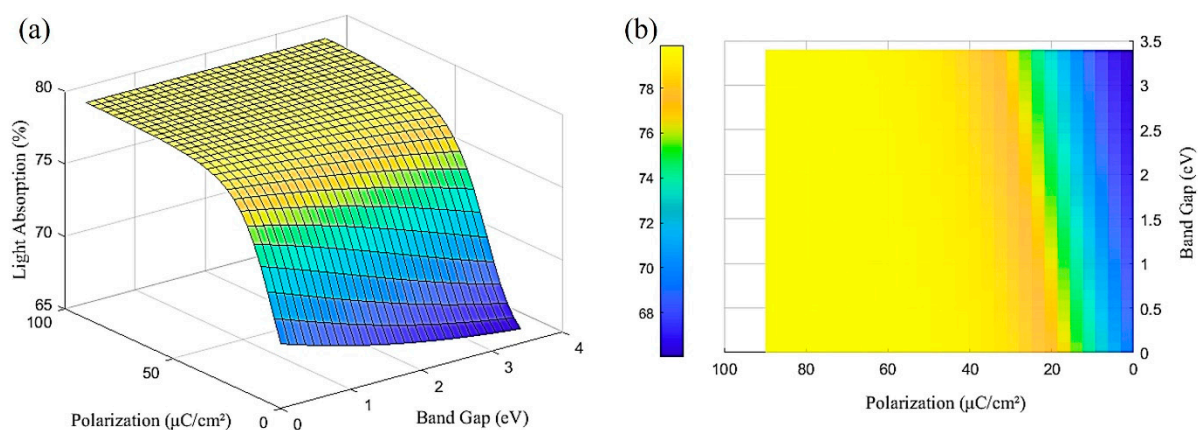


**Figure 8.** Prediction made by the ANN to predict the light absorption of the test object in this study: (a) front view and (b) side view.

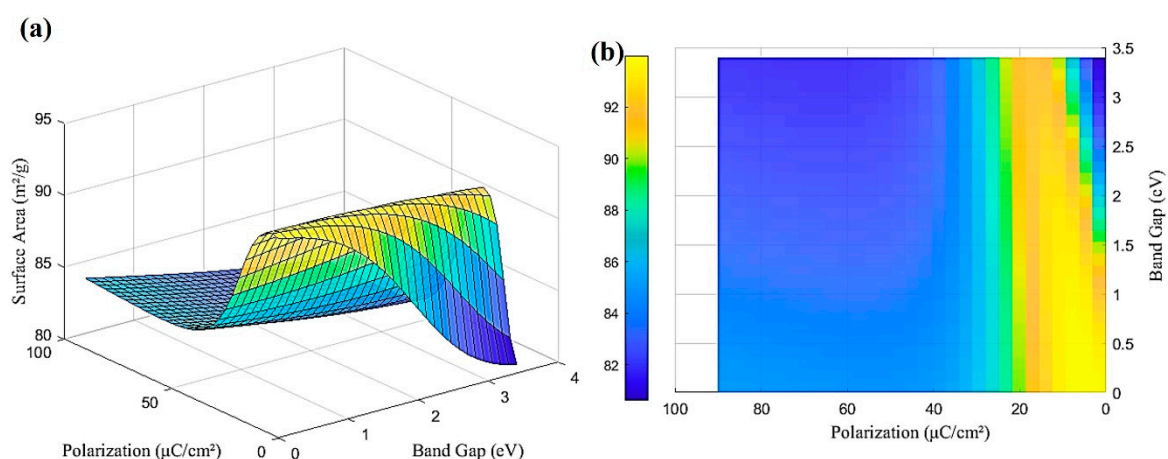


**Figure 9.** Prediction made by the ANN to predict the surface area of the test object in this study: (a) front view and (b) side view.

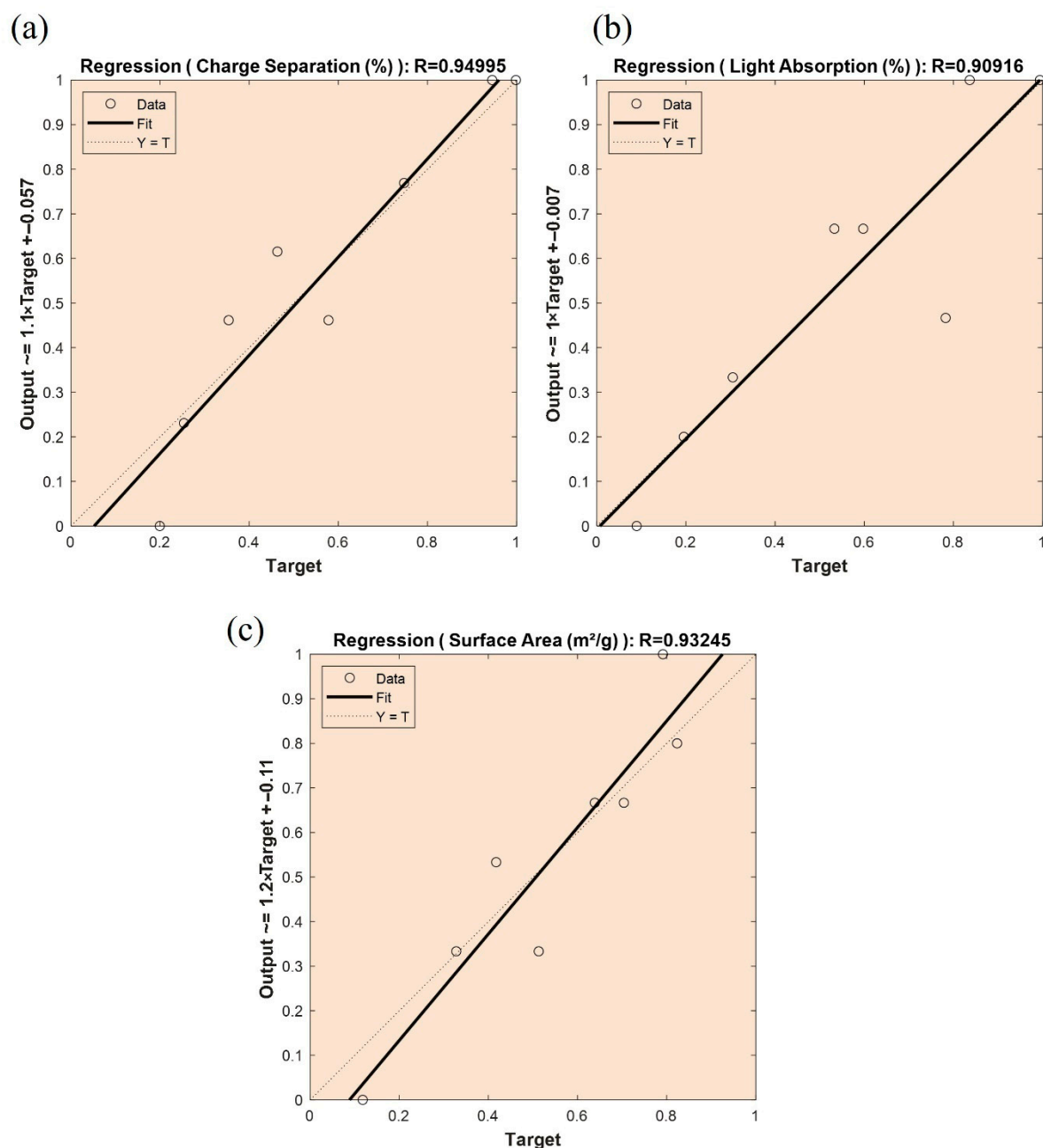


**Figure 10.** Linear regression plots to examine the error of the ANN formed in this study: (a) charge separation (%), (b) light absorption (%), and (c) surface area ( $\text{M}^2/\text{G}$ ).

The captivating light show put on by these ferroelectric materials, with their increasing light absorption as polarization levels rise, has left researchers scratching their heads, as the relationship between polarization and light absorption in these materials can be complex and dependent on factors like electronic structure, band gap, surface properties, and even defects. However, the specific mechanisms driving the intriguing trend seen in Figure 8 remain stubbornly elusive, as if the materials are keeping their secrets closely guarded, refusing to reveal the inner workings that link their polarization to their light-absorbing capabilities. Researchers are thus required to dive deeper, conducting more comprehensive investigations into the interplay between the ferroelectric properties and the photocatalytic performance of these remarkable materials, peeling back the layers of complexity to provide the satisfactory explanations that could unlock new pathways to a greener, more prosperous future by cracking the code of these enigmatic ferroelectric champions.

Ferroelectric materials have emerged as a beacon of hope in the fight against climate change, their unique properties like the ability to switch polarization and improve charge transport making them exceptional photocatalysts for reducing carbon dioxide. By enabling efficient charge separation and transfer during the catalytic process, these materials can dramatically boost the conversion of CO<sub>2</sub> into valuable products. This article delves into the innovative strategies being explored to enhance their surface reactivity, from harnessing polarization effects to engineering nanostructures and defects, as researchers leave no stone unturned in their quest to unlock the full potential of ferroelectrics. As we grapple with the immense challenge of global climate change, the continued progress in this field holds immense promise, with ferroelectric materials leading the charge towards the sustainable solutions we so desperately need to build a greener, more prosperous future for all.

## 7. Conclusions

The use of ANNs holds great promise in advancing the development of ferroelectric photocatalysts for efficient carbon dioxide reduction. ANNs can model the complex relationships between material properties and photocatalytic performance, uncovering non-linear patterns those traditional methods may miss. By training ANN models on experimental and simulation data, researchers can identify optimal material compositions, morphologies, and synthesis conditions to maximize CO<sub>2</sub> conversion. The ANN's ability to handle multidimensional data accelerates the exploration of the parameter space while also providing deeper insights into the underlying charge separation, light absorption, and surface reactivity mechanisms. Integrating ANN-based approaches with experimental and simulation techniques is crucial to realizing the full potential of ferroelectric photocatalysts in addressing climate change. Using ferroelectric materials to reduce carbon dioxide emissions offers an innovative approach to mitigating climate change. Ferroelectric materials have some unique properties that make them valuable for different environmental applications, especially in reducing carbon dioxide levels in the atmosphere. One exciting potential use for these materials is in developing carbon capture and storage technologies. They can help create efficient systems that absorb and store carbon dioxide emissions from factories before they are released into the air, which can significantly lower greenhouse gas emissions and help fight climate change. Plus, ferroelectric materials can also be used in renewable energy technologies like solar panels and wind turbines, contributing to a more sustainable future. By combining these materials in energy harvesting devices, more clean energy is produced and dependence on fossil fuels is reduced, and, as a result, carbon dioxide emissions are reduced. In addition, ferroelectric materials can also play a role in improving energy storage systems such as batteries and capacitors. By increasing the performance of these energy storage devices, renewable energy sources are better integrated into the grid and the overall carbon dioxide emissions associated with electricity production are reduced. As a result, ferroelectric materials have great potential in reducing carbon dioxide emissions and climate change. By using the unique properties of these materials in various environmental applications, we move towards a more sustainable future and combat the challenges of global warming. By changing the band gap (eV) and polarization ( $\mu\text{C}/\text{cm}^2$ ), the parameters of charge separation (%), light absorption (%), and surface area ( $\text{m}^2/\text{g}$ ) can be changed. Charge separation is highest when both the band gap (eV) and polarization ( $\mu\text{C}/\text{cm}^2$ ) are at their lowest levels. Light absorption is maximized when the band gap is at its minimum while polarization is at its highest. Likewise, surface area ( $\text{m}^2/\text{g}$ ) reaches its peak when both the band gap and polarization are at their lowest.

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