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The Study of the Green Synthesis of Y-Doped TiO_2 Nanoparticles for enhancing the performance of Solar Cells

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Abstract

Yttrium (Y)-doped titanium dioxide (TiO_2) nanoparticles have been identified as promising photoanode sources for improving solar cell efficiency due to favorable electronic properties and defect chemistry tunability. This review evaluates the recent literature on Y-doped TiO_2 for use in photovoltaic devices, which focuses particularly on green synthesis methods and the resultant impact on structural, optical, and electronic properties. Y-doping in TiO_2 nanoparticles has been the subject of many studies in the context of dye-sensitized solar cells (DSSCs) and perovskite solar cells (PSCs), but relatively few DSSC studies have applied significant green synthesis principles. Of the literature surveyed, there is only one study that assessed Y doping in TiO_2 while also applying green synthesis principles and measuring device efficiency, and this represents a significant gap in the literature. In recognizing this gap, we have described green synthesis methods that we have categorized as plant extract-based, microbial, and eco-friendly solvothermal, but from literature that employs different dopants or metal oxides. When compared using the same photovoltaic parameters, it is found that the addition of Y to TiO_2 nanomaterials typically has a positive effect on the solar energy conversion efficiency, particularly when exhibiting a combination of desirable morphology and surface chemistry. However, this review reveals that high efficiency devices reported in the literature have only focused on conventional chemical methods, and that material performance about solar energy conversion efficiency is not well connected to principles of sustainability. We recommend more sustainable synthesis in future studies that would lead to less harmful methods of producing materials for future generations.

Keywords
Green Synthesis, Nanoparticles, Solar Cells, Photoanode.

1. Introduction

Titanium dioxide (TiO_2) has been extensively researched as a photocatalyst for solar energy applications due to its desirable photocatalytic properties, relatively stable chemical structure, and abundant natural sources. The bandgap of TiO_2 is relatively wide (~3.2 eV for anatase) and its intrinsic fast electron-hole recombination prevents TiO_2 from absorbing in the visible region (Khan et al., 2013), which ultimately reduces its energy conversion potential, and thus it is important to overcome these inherent limitations.

One particularly attractive mitigation strategy is the introduction of rare earth dopants like yttrium (Y^{3+}) into the TiO_2 lattice. The use of Y as a dopant will be explored at length in this review, as the odd-electron trivalent rare earth ions serve to modify the physicochemical properties of the TiO_2 structure and thus modify its photocatalytic attributes (Nwankwo et al., 2023). While other dopants will also be discussed, rare earth ions can include several distinct properties (i.e., structural, electrochemical, and optical properties) that will allow the synthesized TiO_2 to have oxygen diffusive point defects and minimize competitive recombination losses while shifting the materials bandgap into the visible UV regions. Y doping offers a favorable compromise between compatibility with the Ti^{4+} ionic radius and its stability in the TiO_2 lattice.

The topic of sustainable and green methods of synthesizing doped nanomaterials has gained traction recently as researchers are seeking ways to mitigate the environmental impact of traditional chemical approaches. Green synthesis approaches can also be seen as either completely environmentally friendly or can incorporate plant extracts, microorganisms, or biocompatible reducing agents in their synthesis protocol(Rifat et al., 2025). The use of green synthesis approaches can be a sustainable means, but also sometimes a cheaper way to synthesize doped nanomaterials, while utilizing a potential higher performance item. There has been evidence that Y doped TiO_2 materials made by green synthesis have improved light absorption, improved charge separation, and minimized recombination, thus there is a possible potential for Y doped TiO_2 to be suitable for use in next-generation solar cells (Shobana et al., 2023).

This review article covers a thorough review of the existing green synthesis strategies for Y doped TiO_2 nanoparticles and their physicochemical properties, as well as their impact on solar cells. This review will also cover the development over the last several years in using Y-doped TiO_2 in photonic devices, and touch on the challenges, prospects, and future trends developing Y-doped TiO_2 coated photovoltaic devices and thus improve the researchers' knowledge of developing materials toward practical solar energy applications.

2. TiO_2 Nanoparticles

TiO_2 at the nanoscale has optical and electronic characteristics that are different, compared to its bulk. (De Angelis et al., 2014) The very small nanoparticles can have quantum size effects that change the bandgap and light absorption, and the large surface area increases dye adsorption-which are important in dye-sensitized solar cells (DSSCs). Particles of smaller size (<10 nm) offer more dye-binding surfaces but might enhance grain boundary resistance and electron trapping, where larger particles (>25 nm) offer a higher level of crystallinity and electron transfer but reduces surface area (D. Zhou et al., 2013). Hierarchical systems, e.g. nanoparticles on nanorods or mesoporous films, can be employed to achieve a balance between high dye loading and effective electron pathways to reduce recombination without compromising efficiency of charge transport.

1.1 Synthesis Methods for TiO_2 Nanoparticles

TiO_2 The features of TiO_2 nanostructures are highly dependent on the synthesis route. Synthesis routes are either chemical or non-chemical methods commonly utilized to generate TiO_2 nanoparticles which include:

- **Sol-gel method**: It's a cheap, low-temperature, and chemical-synthesis method that allows for control of particle size and morphology. The sol-gel method relies on the hydrolysis and condensation of titanium alkoxides and may include an optional calcination stage to crystallize the solvent.
- **Hydrothermal/solvothermal synthesis**: A sealed autoclave is utilized at temperature at pressure to yield highly crystalline nanoparticles with uniform morphology and phase purity. Hydrothermal synthesis can form hierarchical structures (e.g. nanorods, nanosheets).
- **Precipitation method**: This route to generating TiO_2 nanoparticles is very simple, low-cost, and quite reproducible for producing suspension of TiO_2 nanoparticles. Precipitation consists of adding a base to a titan salt solution and thoroughly washing and/or heat treat the precipitate.
- **Microwave-Assisted synthesis**: Using microwave-assisted synthesis you are subjected to localized areas of rapid heating and nucleation lead to smaller and more uniform nanoparticles. The microwave-assisted synthesis is becoming more common because it is cost-efficient and a scalable and energy efficient route.
- **Green Synthesis**: Complete waste and lack of toxic chemical agents that may be traditionally utilized to for the generation of TiO_2 nanoparticles by exploiting bio-based agents from natural plant sources, or amino acids, etc. or green chemistry principles. There are many opportunities for eco-friendly means to generate TiO_2 nanoparticles.

1.2 Yttrium as a Dopant

Starting Small particles of pure TiO_2 have a large bandgap (~3.2 eV) and only absorb UV light (~ 5 percent of the solar spectrum), preventing its use as a high-efficiency collector of visible light. Rare earth doping, especially with yttrium (Y^{3+}), can alter its electronic and structural characteristics, to improve photovoltaic activity (Taneja et al., 2024). Effects of Lattice Distortion and Substitution: Ti is bigger (0.605Å) than the Y (0.90Å) and it distorts the lattice resulting in oxygen vacancies, which enhances the separation of charges by lowering the recombination between electrons and holes (K. S. Kumar et al., 2014). Moderate Y-doping (1-5 mol%) stabilizes anatase phase, inhibits the anatase-rutile transformation, decreases the size of particles and increases surface area, which enhances surface adsorption and interfacial contact in DSSCs. Electrical Properties: Y-doping reduces the band gap, raises the Fermi level and enhances the mobility of charge carriers, which enhances electron transport and photocurrent generation (Deng et al., 2019; Khan et al., 2013; Shobana et al., 2023). Optimal Y concentrations (~4–5%) are the point where solar and photocatalytic performance are maximum, and excessive doping hinders performance. Altogether, TiO_2 - based solar cell efficiency can be increased with Y-doping, as well as other element dopants, up to 20 times in the case of the perovskite solar cells (Apostolova et al., 2023). A comparison amongst PCE improvements across dopants is illustrated in Table 1.

Table 1**.** Comparison of power conversion efficiency of different dopants

TiO_2 Dopant	**Synthesis method**	**Undoped PCE (%)**	**Doped PCE (%)**	**Improvement (%)**	**Reference**
Ba	sol-gel	1.29	1.03	-20.16	(Nwankwo et al., 2023)
Cs	sol-gel	1.29	2.81	117.83	(Nwankwo et al., 2023)
Y	sol-gel	1.29	4.5	248.84	(Nwankwo et al., 2023)
Y	-	12.85	19.3	50.2	(H. Zhou et al., 2014)
Zr	hydrothermal	6.6	12.35	87.12	(Qureshi et al., 2021)
Ca	sol-gel	6.53	9.79	49.92	(Arshad et al., 2022)
Bi	-	3.58	5.50	53.63	(Mishra et al., 2025)

3. Applications in Solar Cells

TiO_2 is significant in a variety of solar cells due to its dielectric transparent nature, high mobilities of electrons, and no chemical reactivity. TiO_2 serves as a high surface area scaffolding for dye (and electrons) adsorption for dye sensitized solar cells, but as nanoparticles, TiO_2 serves as an electron transport layer in a perovskite solar cell by utilizing TiO_2 to extract any photogenerated electrons and transport them to the electrode effectively. Silicon based solar cells utilize TIÚ as an anti-reflective coating to improve light absorption. TiO_2 is important to thin film solar cells and quantum dot solar cells as it assists with charge separation and as stabilization of the device itself. All of these various applications utilize TiO_2 to provide efficiency and stability based on improvements made upon the light absorption of the solar technology. (Esmaeili-Zare & Amiri, 2022)

One of the major limitations of TiO_2 for solar applications is the high likelihood of rapid recombination of photogenerated electrons and holes (Weibel et al., 2006). The efficiency of TiO_2-based photoanodes is reliant on conduction band alignment with the redox potential of the dye/electrolyte, through put of electrons in the TiO_2 film, trap states due to oxygen vacancies, grain boundaries, or surface defects.

Pure anatase TiO_2 has reasonable electron diffusion characteristics ($\sim10^{-5}$–10^{-6} cm^2/s); however, this is usually improved through doping or by combining TiO_2 with conductive compounds (e.g. graphene, carbon nanotubes). In addition to morphology (porosity and thickness), thickness modifies recombination and electron transport. Thicker films allow for more dye, but with more dye comes more recombination unless better charge collection has been employed.

1.3 Dye-sensitized solar cells (DSSCs)

A form of third-generation solar cell is the dye-sensitized solar cells (DSSCs) which use dye to capture sunlight and create electrons like photosynthesis. In most cases, it is TiO_2 because it is the most frequently available photoanode material with a high surface area, adequate conduction band alignment with sensitizing dyes, and a known non-toxicity (Awsha et al., 2021; Y. Kumar et al., 2023). Its large band gap (gap of about 3.2 eV in anatase), and slow electron mobility, however, restrict the absorption of light and movement of charge. It has been demonstrated that doping TiO_2 with a rare-earth element, yttrium (Y^{3+}) is an effective way of overcoming these limitations and enhancing the performance of DSSC (Reszczyńska et al., 2015). The typical DSSC set-up is a transparent conducting oxide (TCO) front electrode (FTO or ITO), a high dye adsorption mesoporous layer of TiO_2, a sensitizer dye, to inject electrons into the TiO_2 conduction band, a liquid electrolyte (I^-/I^{3-} redox couple) to regenerate charge, and a counter electrode (Pt or carbon-based) to complete the circuit (Sekaran & Marimuthu, 2023). TiO_2 nanoparticles are used in the DSSCs to enhance the dye loading to enable a high rate of light absorption, a low rate of recombination leading to electron transfer to the anode, and long-term stability of the system during the sunshine.

1.3.1 Y-Doped TiO_2 in DSSCs

The large energy bandgap (~3.2 eV for anatase TiO_2) and low electron mobility of TiO_2 may limit its light absorption ability and charge transport properties.(Dubey et al., 2021) We are exploring doping TiO_2 with yttrium (Y^{3+}), a rare earth element, to improve many of the properties of TiO_2. As indicated in Table 2, all relevant properties of Y-Doped TiO_2 are better than all other rare earth and transition metals.

Certainly, Y^{3+} doping in TiO_2 is very sensitive to doping concentration. (Tobaldi et al., 2013). At low and moderate doping concentrations, Y^{3+} dopants can substitute for Ti^{4+} in the anatase lattice, causing localized lattice distortions that are generally favorable for both electron transport and the adsorption of dyes. However, if the concentration of doping was higher than optimum, this would risk the risk of phase destabilization and growing secondary Y-containing phases (e.g., Y_2O_3); this would also risk limiting the ability for light-harvesting, thereby increasing charge recombination. In the laboratory, previous literature had established a general range of optimum Y^{3+} doping be considered at 0.5–2 mol% in terms of providing a good balance between structural integrity and improved performance in dye-sensitized solar cells (DSSCs). Usually in this range kept the anatase phase of TiO_2 and enhanced the performance because of incorporation of beneficial oxygen vacancies and defect sites positioning favorable for charge separation, while maintaining adequate surface area for dye anchoring.

Research studies also provide evidence that the strict upper limit on Y doping is highly variable. As an example, Y-doped TiO_2 prepared by a 'green' solvothermal route and utilizing glycerol as a ligand has been reported to have performance enhancements, (even at 5 mol% Y), with published data indicating a power conversion efficiency of 6.88%, which is higher than both undoped and lower-doped Y material, plus there were no evidence of any secondary phase transitions; this suggests that preparation method may have a key role to stabilize the anatase phase of TiO_2 where relatively larger concentrations of dopants are used to synthesize the TiO_2 (Shobana et al., 2023).

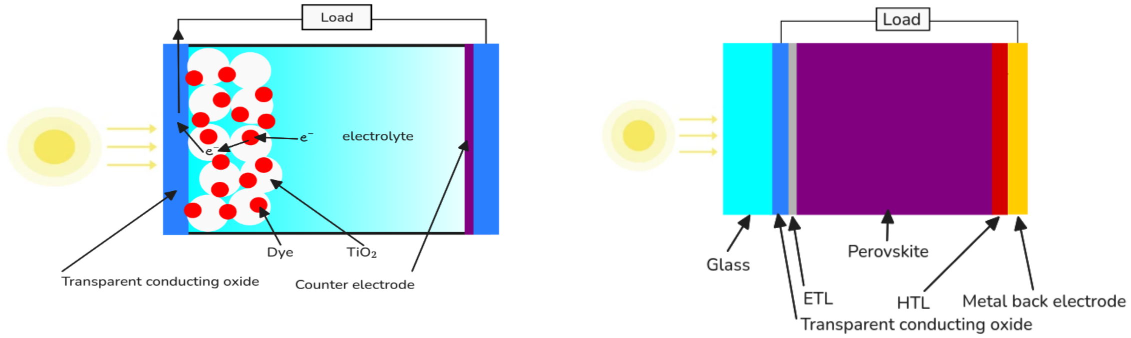
Table 2**.** Photovoltaic parameters of various doped TiO_2 based DSSC

Photoanode	V_{OC} **(V)**	$J_{SC}\ (mA - cm^{-2})$	**Fill Factor (%)**	**PCE without doping (%)**	**PCE (%)**	**Reference**
TiO_2	0.67	10.62	51.9	3.7	3.7	(Chappidi et al., 2024)
Er-TiO_2	0.72	15.03	61.4	3.7	6.7	(Chappidi et al., 2024)
Sm-TiO_2	0.71	14.28	61.1	3.7	6.2	(Chappidi et al., 2024)
Nd-TiO_2	0.68	13.58	58.4	3.7	5.4	(Chappidi et al., 2024)
Yb-TiO_2	0.69	14.06	50.5	3.7	4.9	(Chappidi et al., 2024)
Y-TiO_2	0.715	15.27	63.01	-	6.88	(Shobana et al., 2023)
Fe-TiO_2	0.65	2.91	55	-	1.11	(Nikhil et al., 2024)
Ni-TiO_2	0.786	10.15	45	2.51	3.60	(Raguram & Rajni, 2021)
Co/rGO-TiO_2	0.618	12.83	-	3.71	5.24	(Ahmad et al., 2022)

1.4 Perovskite Solar Cells

Perovskite solar cells are a developing thin-film photovoltaic technology, whose materials are described by the general formula ABX_3, where A is an organic or inorganic cation, B a metal cation (typically Pb^{2+} or Sn^{2+}), and X a halide anion. The characteristics of these materials are a direct band gap with a tunable band gap of between 1.2-2.3 eV, large absorption coefficients and long carrier diffusion lengths which facilitate easy absorption of light using very thin absorber layers. Perovskite solar cells have already demonstrated quick improvements in efficiency with laboratory cells reaching an efficiency of more than 25 percent power conversion, on a par with crystalline silicon solar cells.

They are among the most promising next-generation PV technologies due to their compatibility with low-cost solution processing, and the capability to be configured in tandem architecturesn (Figure 1).



(a) (b)

Figure 1. (a)Working principle of DSSC (b) Working principle of PSC

1.4.1 Y-Doped TiO_2 in in PSCs

PSC efficiency is often limited by charge losses and stability issues, both of which can be improved using Y-doped TiO_2. Research has shown that optimized Y doping can lead to higher power conversion efficiency (PCE) and better moisture stability in perovskite devices (Deng et al., 2019; Nwankwo et al., 2023).

Y^{3+} ions, when incorporated into the TiO_2 lattice, can induce several beneficial effects:

- **Improved charge transport**: Y doping increases carrier mobility and conductivity by introducing shallow donor levels or by passivating trap states in the TiO_2 matrix.
- **Reduced recombination losses**: Y^{3+} doping can modify surface states and improve energy-level alignment at the ETL/perovskite interface, thereby lowering interfacial recombination.
- **Enhanced stability**: Some studies have shown that Y-doped TiO_2 improves the moisture and thermal stability of PSCs by creating a more compact and less reactive ETL surface.
- **Morphological improvements**: Doping can influence grain growth in the perovskite layer deposited atop the ETL, indirectly improving film uniformity and interface contact.

2. Experimental Evidence and Limitations

The experimental work on Y-doped TiO_2 as a compact electron transport layer (c-TiO_2) in perovskite solar cells (PSCs) demonstrated notable enhancements on photovoltaic performance. Nwankwo et al.(Nwankwo et al., 2023) used a two-step sequential deposition process to develop PSCs using pure TiO_2 and p-type metal doped TiO_2 (Ba, Cs and Y) as the ETL on patterned fluorine doped tin oxide (FTO) glass substrates with a number of different deposition amounts and/or compositions. X-ray diffraction (XRD) work confirmed the doping of the TiO_2 to use in the PSCs, as evidenced by an increase in the c-axis of the TiO_2 lattice parameter and reduction in crystallite size indicating that doping by the metal occurred within the TiO_2 lattice to incorporate into the tetragonal structure of the TiO_2.

Y-doped TiO_2 was proven to be the best performing dopant, with an average power conversion efficiency (PCE) of 4.25% and a maximum of 4.50% to compare to undoped TiO_2 which gave an overall average PCE for its devices of 1.69%. Ba- and Cs-doped TiO_2 gave lower average efficiencies overall (with Ba-doped TiO_2 and average of (0.96% and Cs-doped TiO_2 with an average of 1.92%), and this is likely due to the better J_{SC} and V_{OC} of the Y-doped devices indicating better charge separation and less charge recombination at the ETL/perovskite interface.

While this paper adds to the literature on Y-doped TiO_2, only a small number of previous studies or Y-doped TiO_2 done by green synthesis principles, and most studies use the conventional hazardous sol-gel or hydrothermal synthesis route with hazardous solvent source and for the metal dopant to be complexing agent source. Furthermore, Y-doped TiO_2 has yet to be compared across multiple different perovskite compositions and spherical vs planar or mesoporous devices.

5. Conclusion

Yttrium (Y) doping of TiO_2 nanoparticles has been demonstrated to be effective in improving solar cell technologies and in particular dye-sensitized and perovskite solar cells by increasing their conductivity, charge separation, and stability thereby raising their power conversion efficiency. Although green synthesis of Y -TiO_2 with plant extracts or microorganisms is in line with sustainable materials science, studies with Y doping, green synthesis, and device construction are scarce. The existing literature demonstrates that there is no universal tendency in the performance of dopants, and optimization is based on cases. The future includes the expansion of green synthesis, the potential of Y to be used with other dopants as well as the expansion of photovoltaic testing to create efficient, durable, and sustainable solar energy systems.

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