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Green Synthesis Of Metal Oxide Nano-Catalysts For CO_2 Reduction And Water Purification

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Abstract:

The increasing levels of atmospheric carbon dioxide (CO_2) and widespread water contamination have emerged as critical global environmental challenges. In this research paper, the development of eco-friendly and cost-effective catalytic systems is essential for sustainable remediation strategies. This study focuses on the green synthesis of metal oxide (TiO_2) nano-catalysts using plant extracts *Ocimum sanctum* alternative to conventional chemical methods. The synthesized nano-catalysts, TiO_2, were characterized using XRD, SEM and TEM, techniques to evaluate their structural and morphological properties.

The green-synthesized nano-catalysts demonstrated excellent catalytic activity in two key applications: photocatalytic CO_2 reduction under simulated solar light, and degradation of organic pollutants in wastewater. The CO_2 reduction experiments showed enhanced conversion efficiency toward valuable products such as methanol and formic acid, while water purification trials exhibited significant degradation rates of dyes and pharmaceutical contaminants. The performance is attributed to the high surface area, controlled morphology, and enhanced charge separation of the green-synthesized nanomaterials.

Keyword: Photocatalyst, SEM, TEM, XRD, Pollutant, Nano-catalyst etc.

Introduction

A fundamental human right, access to safe drinking water is becoming more and more challenging due to pollution and water scarcity worldwide [1]. Only 0.3% of the 8.1 billion people on Earth have access to freshwater, despite the fact that two-thirds of the planet's surface is covered by water. As freshwater resources are exhausted, human activities are at risk due to water scarcity. With 1.2 billion people receiving only minimal water services and 2 billion people needing safe water, current water treatment facilities are unable to keep up with the expanding demand [2,3]

The continuous advancement of industrial activities, coupled with the rapid growth of the global population, has led to an exponential rise in the release of chemical pollutants into aquatic ecosystems, resulting in significant deterioration of water quality.[4]

This challenge has spurred efforts to enhance and optimize water treatment processes, aiming to maximize pollutant removal efficiency while minimizing energy and chemical consumption. However, many contaminants—particularly emerging contaminants (ECs) are resistant to conventional treatment methods such as membrane separation, chemical oxidation, ion exchange, biological processes, activated carbon adsorption, and ozonation. ECs are a class of largely unregulated and relatively understudied compounds that may pose significant risks to human health and the environment.[5]

Green chemistry emerged as a distinct scientific discipline in the United States during the 1990s. Since then, European countries have taken the lead in implementing advanced regulations promoting green technologies. In recent years, novel reaction pathways and environmentally conscious processes have been developed to significantly reduce the environmental impact of chemical production, particularly by minimizing the use of hazardous substances and the generation of harmful by-products [6].

Currently, green chemistry is advancing along three primary fronts: the development of new synthetic methods utilizing catalysts; the replacement of traditional organic solvents, notably through the use of supercritical CO_2; and the adoption of renewable feedstocks, such as non-petroleum-based reagents [7].

Green magnetic nanoparticles, in particular, exhibit low toxicity and high biocompatibility, making them suitable for biomedical applications such as targeted drug delivery, contrast imaging, and magnetic hyperthermia. The structure and morphology of synthesized magnetic nanoparticles can be characterized using techniques such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Fourier-transform infrared (FTIR) spectroscopy, Raman spectroscopy, and magnetic force microscopy (MFM). MFM, a highly sensitive technique capable of detecting weak magnetic fields with a resolution of up to 10 nm, is widely used for analyzing magnetic nanoparticles due to its minimal sample preparation requirements and its versatility in operating under air, vacuum, or liquid environments [8].As clean drinking water becomes more scarce, water filtration technologies are becoming more and more popular worldwide. Cost-effective, energy-efficient solutions require sustainable breakthroughs. Long-term potential is presented by nanotechnology, which can lower prices, improve water quality, and improve filter materials. A major factor in these developments are nanomaterials, which are materials created at the nanoscale (less than 100 nanometres). Because of their special qualities, nanomaterials like graphene oxide (GO) and carbon nanotubes (CNTs) are useful for purifying water [9].

This research paper focuses on green metal oxide nano-catalysts synthesis and their application in Co_2 reduction and water purification.

1. Materials and methods:

1.1 Eco-friendly method for preparation of TiO_2 Nano-catalyst:

There are several methods by using plants and microorganisms, such as algae, bacteria, fungi, viruses, yeasts, and waste materials, as well as combining these biogenic processes with alternative activation methods like microwave and ultrasound, there are a number of environmentally friendly and biological ways to create nanomaterials [10]. The production of sustainable nanostructures, such as nanoflowers, nanowires, nanorods, nanotubes, and nanoparticles, is aided by the presence of flavonoids, terpenoids, proteins, vitamins, phenolic acid, glycosides, carbohydrates, polymers, alkaloids, and different antioxidants[11].

Ocimum sanctum, also known as Tulsi or Holy Basil, is a highly valued medicinal plant in Ayurveda, Unani, and folk medicine. It has been used for thousands of years in India for its diverse therapeutic properties, owing to its rich content of essential oils, flavonoids, and polyphenols. The green synthesis of metal oxide nanoparticles using Ocimum sanctum (tulsi) plant extracts involves a simple, eco-friendly process. First, a plant extract is prepared by boiling Tulsi plant parts such as leaves, bark, or fruit peels in distilled water to release bioactive compounds like Eugenol, tannins and flavonoids which act as reducing agent. After filtration, the extract is mixed with a metal precursor solution, titanium isopropoxide for TiO_2. This mixture is then stirred and gently heated, allowing the phytochemicals present in the extract to act as natural reducing and stabilizing agents, facilitating the formation of nanoparticles. The resulting product is dried to remove moisture and subsequently calcined at high temperatures to enhance crystallinity and obtain pure, stable metal oxide i.e.Tio_2 nanoparticles.

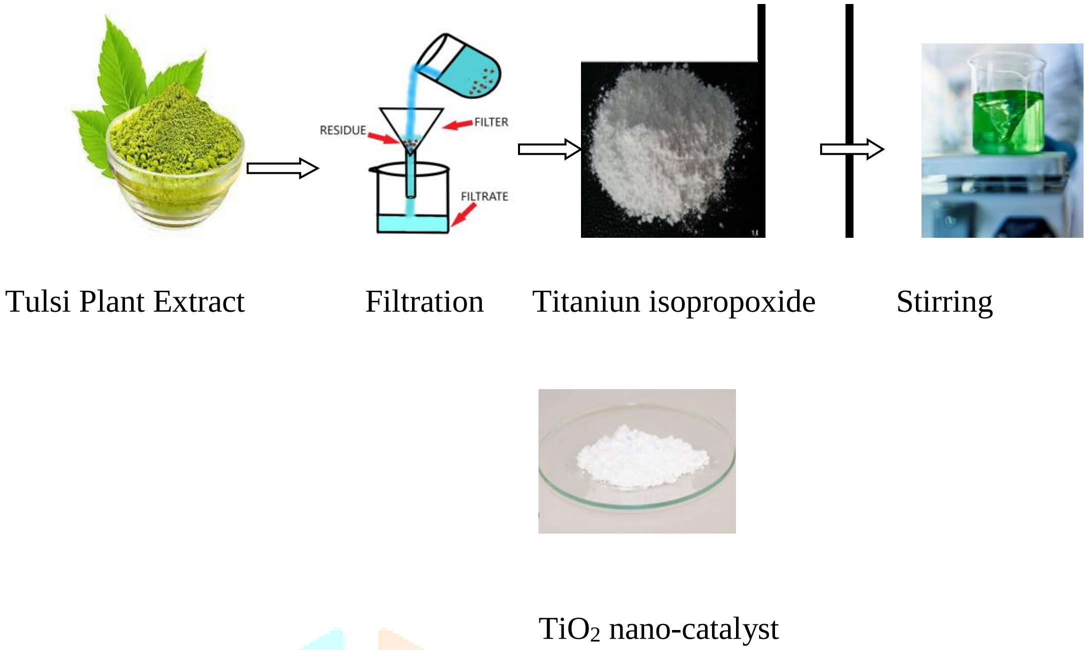

Figure-1: Schematic representation of TiO_2 NPs synthesized using plant extract.

2. Characterization of TiO_2 nanao-catalyst:

2.1 SEM Analysis : SEM (Scanning Electron Microscopy**)** is a powerful technique used to study the surface morphology and topography of materials at the nanoscale[12]. The SEM images of the synthesized TiO_2 nanoparticles revealed a predominantly spherical morphology with average particle sizes ranging from 20 to 40 nm. Some degree of agglomeration was observed, likely due to the high surface area and Van der Waals forces between particles. The uniformity in shape suggests effective synthesis using the green method.

2.2 TEM Analysis : TEM (Transmission Electron Microscopy) is a high-resolution technique used to observe the internal structure**,** size**,** shape, and crystallinity of nanoparticles at the atomic or nanometer scale. TEM analysis of TiO_2 nanoparticles synthesized using *Ocimum sanctum* extract at 200 kV showed predominantly spherical particles with an average size of 25 nm. The particles were well-dispersed with some minor agglomeration. High-resolution images revealed clear lattice fringes, confirming the crystalline nature of the anatase phase of TiO_2.

2.3 X-ray diffraction: XRD analysis of the TiO_2 nanoparticles synthesized using Ocimum sanctum extract, carried out at 40 kV and 200 µA using Cu Kα radiation, revealed sharp diffraction peaks at 2θ values of 26.34°, 36.7°, 46.0°, 55.8°, 55.1°, and 64.8°, corresponding to the (102), (005), (200), (106), (212), and (203) planes of anatase TiO_2[13]. The average crystallite size was calculated to be 32.7 nm using the Scherrer equation. The absence of peaks corresponding to rutile or brookite phases confirmed the high phase purity of the synthesized nanoparticles."

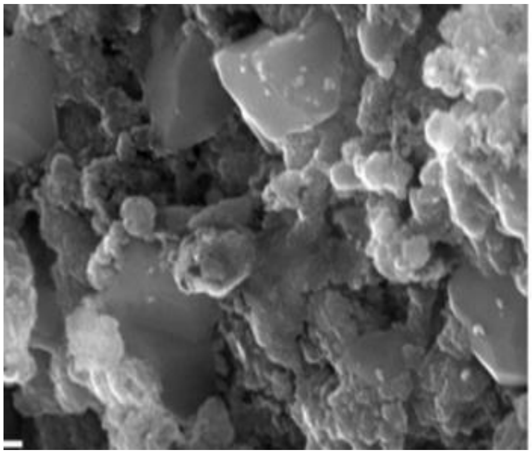

Figure-2: SEM image of TiO_2 at 1 mu

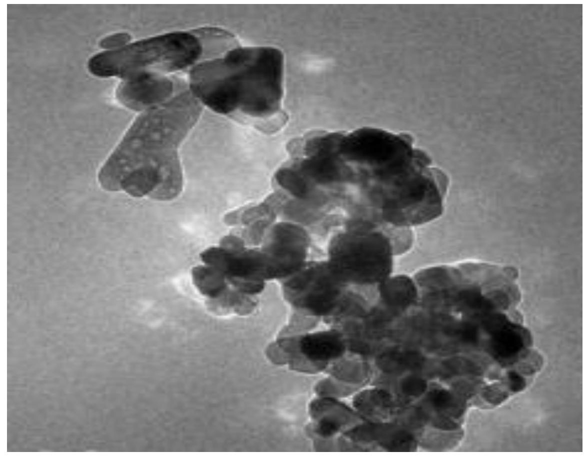

Figure-3 : TEM images of TiO_2 at 200 mu

3. Result and Discussion :

3.1 Use of TiO_2 Nanoparticles in Water Purification:

Titanium dioxide (TiO_2) nanoparticles are widely recognized for their exceptional ability to purify water through a process known as photocatalysis[14]. This advanced oxidation process relies on the unique semiconductor properties of TiO_2, particularly when it is exposed to ultraviolet (UV) light. Upon UV illumination, TiO_2 nanoparticles absorb photons with energy equal to or greater than their band gap (about 3.2 eV for anatase phase), resulting in the excitation of electrons from the valence band to the conduction band. This creates electron-hole pairs (e^-/h^+) that are highly reactive.

These charge carriers initiate a series of redox reactions at the surface of the TiO_2 particles. The photo-generated holes (h^+) can oxidize water (H_2O) or hydroxide ions (OH^-) to produce hydroxyl radicals (•OH) extremely reactive and non-selective oxidizing agents. Simultaneously, the photo-generated electrons (e^-) reduce dissolved oxygen (O_2) to form superoxide radicals ($O_2{\bullet}^-$). These reactive oxygen species (ROS) play a central role in breaking down a wide range of organic pollutantsie. Atrazine, Paracetamol, Diclofenac, including dyes ie. Methylene blue, Rhodamine B, Congo red, pharmaceuticals ie. , pesticides, and microbial contaminants. The pollutants are ultimately mineralized into harmless end products such as carbon dioxide (CO_2), water (H_2O), and inorganic ions.

In addition to degrading chemical contaminants, TiO_2 nanoparticles exhibit antibacterial properties**.** The ROS generated during photocatalysis cause oxidative damage to microbial cell walls, leading to the inactivation or death of bacteria and viruses. This makes TiO_2 an effective multifunctional agent for both chemical and biological purification of water.

TiO_2 nano-catalyst is highly favored for water treatment because it is non-toxic, chemically stable, inexpensive, and reusable. However, its effectiveness is limited under visible light due to its wide band gap. To overcome this, modifications such as doping with metals (e.g., Ag, Fe) or non-metals (e.g., N, C) have been employed to enhance its activity under visible light.

3. 2 Use of TiO_2 Nanoparticles in CO_2 Reduction :

Titanium dioxide (TiO_2) nanoparticles have gained significant attention in recent years for their role in the photocatalytic reduction of carbon dioxide (CO_2), a promising approach to mitigate greenhouse gas emissions and combat climate change[15]. The process mimics natural photosynthesis, where TiO_2 acts as a photocatalyst to convert CO_2 into useful hydrocarbon fuels such as methane (CH_4), methanol (CH_3OH), carbon monoxide (CO), and other low-carbon compounds[16-17]. This transformation is driven by light energy, typically ultraviolet (UV) light, although efforts are ongoing to improve visible-light responsiveness through doping and surface modification.

When TiO_2 is irradiated with UV light, electrons in the valence band are excited to the conduction band, leaving behind positive holes. These electron-hole pairs (e^-/h^+) initiate redox reactions at the catalyst surface. The conduction band electrons participate in the reduction of CO_2 molecules adsorbed on the TiO_2 surface, while the valence band holes oxidize water molecules to provide protons (H^+) needed for the reduction reactions. The overall process is influenced by several factors, including the surface area of the TiO_2, crystal structure the presence of co-catalysts (e.g., Pt, Cu), and reaction conditions such as pH, temperature, and CO_2 pressure.

A key challenge in CO_2 photoreduction is the activation of the highly stable CO_2 molecule, which requires efficient charge separation and strong surface interaction with the catalyst. TiO_2's large band gap (~3.2 eV) limits its activity to UV light, which comprises only a small fraction of the solar spectrum. To improve its efficiency under natural sunlight, researchers have developed modified TiO_2 nanomaterials through metal or non-metal doping, heterojunction formation, and surface sensitization. These modifications help to narrow the band gap, increase light absorption in the visible range, and enhance the separation of charge carriers.

4.Conclusion and Future perspectives:

The green synthesis of titanium dioxide (TiO_2) nanoparticles offers a sustainable and eco-friendly approach to producing highly functional metal oxide nanomaterials for environmental remediation applications, particularly CO_2 reduction and water purification. By utilizing plant extracts such as those from *Ocimum sanctum* as natural reducing and stabilizing agents, this method avoids the use of toxic chemicals and energy-intensive processes, aligning with the principles of green chemistry.

Green-synthesized TiO_2 nanoparticles exhibit excellent photocatalytic activity due to their controlled morphology, nanoscale size, and the presence of bioactive phytochemicals that may enhance surface properties. In CO_2 reduction, these nanoparticles serve as efficient photocatalysts that convert carbon dioxide into valuable hydrocarbons or fuels under UV or sunlight exposure. Simultaneously, in water purification, TiO_2 facilitates the breakdown of organic pollutants and the disinfection of harmful microorganisms by generating reactive oxygen species upon photoactivation.

Overall, green synthesis not only reduces environmental and health risks during nanoparticle production but also enhances the photocatalytic performance of TiO_2 in real-world applications. This dual-functionality underscores the potential of green-synthesized TiO_2 as a powerful and sustainable material for combating environmental pollution and supporting clean energy solutions.

Future research should focus on integrating these strategies to develop multifunctional, stable, and environmentally benign nanocatalysts for real-world applications.

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