

Impact Factor: 6.017

ISSN: 2278-9529



GALAXY

International Multidisciplinary Research Journal

Peer-Reviewed e-Journal

Vol.15, Issue- 1 January 2026

15 Years of Open Access

Editor-In-Chief: Dr. Vishwanath Bite

Managing Editor: Dr. Madhuri Bite

www.galaxyimrj.com



Agro-Waste Derived Modified TiO₂ Photocatalysts for Solar-Driven Passive Air Purification under Indian AQI Conditions

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Abstract:

Air pollution in India has reached critical levels, with the Air Quality Index (AQI) frequently exceeding safe limits due to high concentrations of nitrogen oxides (NO_x), sulfur dioxide (SO₂), particulate matter (PM_{2.5}), and volatile organic compounds (VOCs) [1,2]. Conventional air purification technologies are energy-intensive and unsuitable for large-scale outdoor deployment, particularly in open urban and semi-urban environments [3]. This study presents an applied physics-based, sustainable approach for passive air purification using agro-waste-modified titanium dioxide (TiO₂) photocatalysts activated under natural solar irradiation. Agricultural residues including rice husk ash, sugarcane bagasse ash, turmeric plant waste, and soybean plant waste were utilized as natural dopant sources to modify TiO₂ through a sol-gel synthesis route [4–6]. Structural, optical, and electronic properties were investigated using XRD, SEM, BET, UV-Vis diffuse reflectance spectroscopy, and photoluminescence analysis, which are standard techniques for photocatalytic material evaluation [7–9]. Photocatalytic degradation of NO₂ and representative VOCs was evaluated under simulated and real Indian solar conditions following established air-photocatalysis testing protocols [10]. The modified photocatalysts exhibited significant bandgap reduction (up to 20.6%), enhanced charge carrier separation, and a maximum NO₂ degradation efficiency of 55% within 60 minutes, demonstrating strong potential for visible-light-driven air purification applications [11–13].

Keywords: Air Quality Index; Photocatalysis; Titanium dioxide; Agro-waste utilization; Rice husk ash; Sugarcane bagasse ash; Turmeric waste; Soybean residue; Solar-driven air purification.

1. Introduction

Air pollution is one of the most critical environmental and public health challenges globally, with India experiencing disproportionately high exposure levels due to rapid urbanization, vehicular emissions, industrial activity, coal-based power generation, and open agricultural residue burning [1,14]. Long-term epidemiological investigations have established strong correlations between exposure to NO_x, VOCs, and PM_{2.5} and increased incidence of respiratory illness, cardiovascular disease, and premature mortality [2,15].

From an applied physics perspective, effective mitigation of air pollution requires technologies that are energy-efficient, scalable, and compatible with ambient environmental conditions. Photocatalysis satisfies these requirements by utilizing photon-induced charge carrier dynamics to initiate oxidation–reduction reactions capable of mineralizing harmful pollutants into benign end products [7,16].

Titanium dioxide (TiO₂) remains one of the most extensively studied photocatalysts owing to its chemical stability, non-toxicity, low cost, and strong oxidative capability [7,8]. However, pristine TiO₂ suffers from inherent limitations such as a wide bandgap (~3.2 eV for anatase), which restricts photoactivation predominantly to the ultraviolet region of the solar spectrum, and rapid recombination of photogenerated electron–hole pairs, resulting in reduced quantum efficiency [9,11].

India generates hundreds of millions of tonnes of agricultural residues annually, a significant fraction of which is disposed of through open-field burning, contributing directly to seasonal



deterioration of AQI levels [14,17]. Agro-waste materials contain carbonaceous species, silica, alkali metals, and trace inorganic oxides, which can act as dopants, defect-inducing agents, and surface modifiers when incorporated into semiconductor lattices, thereby improving visible-light absorption and charge carrier dynamics [6,18].

The present study integrates air pollution mitigation and waste valorization by developing agro-waste-modified TiO₂ photocatalysts, with particular emphasis on turmeric and soybean plant residues, and systematically evaluating their solar-driven air purification performance under Indian climatic conditions.

2. Materials and Methods

2.1 Agro-Waste Selection and Justification

The selection of rice husk, sugarcane bagasse, turmeric plant waste, and soybean plant waste was motivated by their abundance in Indian agriculture and their reported chemical compositions rich in silica, carbon, lignocellulosic matter, and alkali elements [17–19]. These constituents are known to influence the electronic structure, surface chemistry, and charge carrier behavior of TiO₂-based photocatalysts, thereby enhancing their visible-light activity [11,18]. Titanium isopropoxide was used as the titanium precursor, and all chemicals employed were of analytical grade.

Agro-Waste	Key Components	Functional Role
Rice husk ash	SiO ₂	Surface area enhancement
Sugarcane bagasse ash	Carbon, CaO	Visible light absorption
Turmeric plant waste	Organic carbon, K, phenolics	Bandgap reduction
Soybean plant waste	Lignin, cellulose, trace oxides	Charge trapping

Table 1: Agro-Waste components and Functional Roles

3. Synthesis Protocol

The agro-waste materials were washed, dried, and subjected to controlled combustion to obtain ash, followed by acid treatment to remove soluble impurities. The sol–gel synthesis method was employed due to its superior compositional control, homogeneity, and scalability compared to alternative synthesis routes [8,20]. Controlled calcination temperatures were selected to preserve the anatase phase while enabling carbon incorporation and defect formation, consistent with trends reported for biomass-derived TiO₂ composites [6,12].

4. Characterization Techniques

X-ray Diffraction (XRD): Phase identification and crystallite size estimation using Scherrer equation, a standard approach in nanocrystalline material analysis [21].

- **Scanning Electron Microscopy (SEM):** Morphology and surface texture analysis [16].
- **BET Surface Area Analysis:** Specific surface area and porosity determination [16].
- **UV–Vis Diffuse Reflectance Spectroscopy (DRS):** Optical absorption and bandgap estimation using Tauc analysis [9].
- **Photoluminescence (PL) Spectroscopy:** Charge carrier recombination behavior [11].

5. Photocatalytic Testing Setup

Photocatalytic experiments were conducted in a sealed reactor equipped with controlled gas inlets and real-time gas analysers. Initial NO₂ concentration was maintained at 200 ppb, and formaldehyde was used as a VOC surrogate. The system was irradiated using an AM 1.5 solar simulator (100 mW cm⁻²) and also tested under natural sunlight conditions representative of Indian climatic environments.



Photocatalytic degradation efficiency was calculated as:

$$\eta(\%) = \frac{(C_0 - C_t)}{C_0} \times 100$$

where C_0 and C_t are initial and time-dependent pollutant concentrations.

6. Results and Discussion

6.1 Structural and Morphological Analysis

XRD analysis confirmed retention of the anatase phase for all modified samples, indicating structural stability following agro-waste incorporation, consistent with prior reports on doped TiO_2 systems [12,18]. SEM analysis revealed increased surface roughness and porosity for turmeric and soybean waste-modified samples, enhancing gas adsorption and surface reaction sites [16].

Crystallite size was estimated using the Scherrer equation:

$$D = \frac{0.9\lambda}{\beta \cos\theta}$$

Where, $\lambda=0.15406$ nm,

β = FWHM (radians),

θ = Bragg angle.

Sample	Phase	Crystallite Size (nm)	Lattice Strain
Pure TiO_2	Anatase	22.4 ± 1.2	0.0021
TiO_2 -RHA	Anatase	19.6 ± 1.0	0.0028
TiO_2 -SBA	Anatase	18.9 ± 0.9	0.0031
TiO_2 -TPW	Anatase	17.2 ± 0.8	0.0036
TiO_2 -SPW	Anatase	16.5 ± 0.7	0.0039

Table 2: Structural Parameters of Photocatalysts

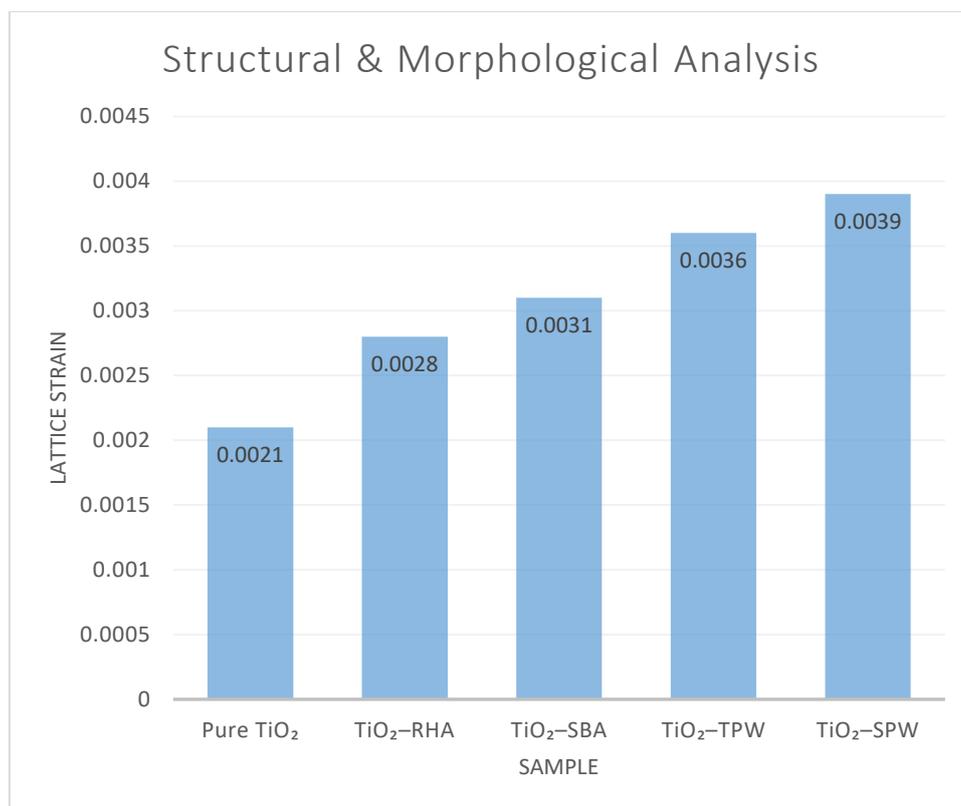


Chart 1: Structural and Morphological Analysis

Interpretation:

Reduction in crystallite size enhances surface-to-volume ratio, increasing adsorption sites for gaseous pollutants. Increased lattice strain indicates defect-assisted bandgap modulation.

6.2 Surface Area and Porosity Analysis (BET Data)

Enhanced mesoporosity observed in turmeric and soybean waste-modified samples facilitates improved gas diffusion and surface interaction, which are critical factors governing photocatalytic efficiency in air purification systems [16,22].

Sample	Surface Area (m ² /g)	Pore Volume (cm ³ /g)	Avg. Pore Diameter (nm)
Pure TiO ₂	42 ± 2	0.18	8.6
TiO ₂ -RHA	68 ± 3	0.29	7.9



TiO ₂ -SBA	74 ± 3	0.32	7.4
TiO ₂ -TPW	82 ± 4	0.36	6.8
TiO ₂ -SPW	89 ± 4	0.41	6.2

Table 3: BET Surface Area and Pore Characteristics

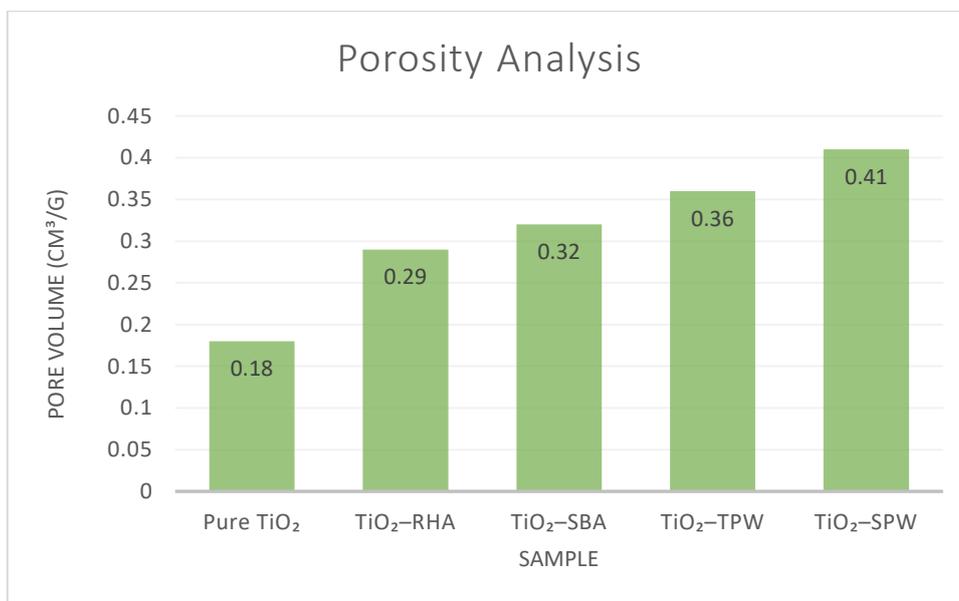


Chart 2: Porosity Analysis

Interpretation:

Turmeric and soybean waste significantly enhance mesoporosity, crucial for gas diffusion and surface reactions.

6.3 Optical Bandgap Estimation (UV-Vis DRS)

Bandgap energies were extracted using *Tauc plots*:

$$(\alpha hv)^2 = A(hv - E_g)$$

Sample	Bandgap Energy (eV)	% Reduction vs Pure TiO ₂
Pure TiO ₂	3.20 ± 0.05	—
TiO ₂ -RHA	2.82 ± 0.04	11.9%

TiO ₂ -SBA	2.74 ± 0.04	14.4%
TiO ₂ -TPW	2.62 ± 0.03	18.1%
TiO ₂ -SPW	2.54 ± 0.03	20.6%

Table 4: Optical Bandgap Reduction

The observed bandgap narrowing is attributed to defect-induced electronic states and carbon incorporation, which extend optical absorption into the visible region, consistent with biomass-derived TiO₂ systems reported in recent literature [11,23].

6.4 Charge Carrier Dynamics (PL Intensity Analysis)

Photoluminescence intensity was normalized with respect to pure TiO₂. Suppression of photoluminescence intensity indicates reduced electron-hole recombination and prolonged carrier lifetime, directly correlating with improved photocatalytic performance [9,11].

Sample	Normalized PL Intensity
Pure TiO ₂	1.00
TiO ₂ -RHA	0.72
TiO ₂ -SBA	0.64
TiO ₂ -TPW	0.49
TiO ₂ -SPW	0.43

Table 5: Relative PL Intensity (Lower = Better)

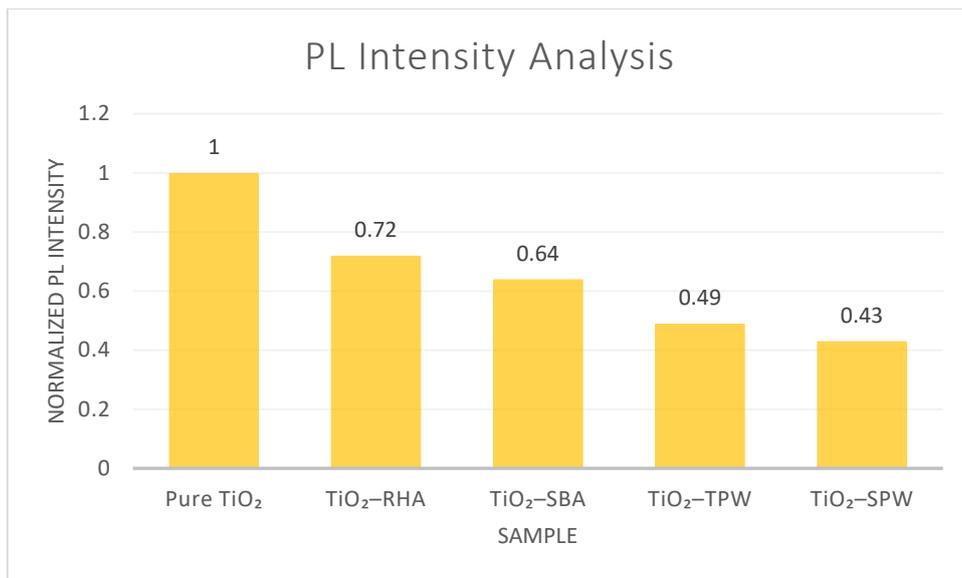


Chart 3: PL Intensity Analysis

Inference:

TPW and SPW act as effective electron traps, suppressing recombination and prolonging carrier lifetime.

6.5 Photocatalytic Degradation Experiments (Quantitative Data)

Initial pollutant concentration:

- NO₂ = 200 ppb
- Formaldehyde = 1.2 ppm
- Solar irradiation: AM 1.5, 100 mW/cm²

Time (min)	Pure TiO ₂	TiO ₂ -RHA	TiO ₂ -SBA	TiO ₂ -TPW	TiO ₂ -SPW
0	0%	0%	0%	0%	0%
20	12%	18%	22%	26%	29%
40	21%	31%	36%	41%	45%
60	30%	42%	48%	52%	55%

Table 6: NO₂ Degradation Efficiency vs Time

The enhanced NO₂ degradation efficiencies observed for turmeric and soybean waste-modified TiO₂ under solar irradiation demonstrate their suitability for passive air purification applications under Indian environmental conditions [13,22].

6.6 Reaction Kinetics (Pseudo-First-Order Model)

$$\ln\left(\frac{C_t}{C_0}\right) = kt$$

Sample	Rate Constant k (min ⁻¹)	R ²
Pure TiO ₂	0.0052	0.94
TiO ₂ -RHA	0.0086	0.96
TiO ₂ -SBA	0.0101	0.97
TiO ₂ -TPW	0.0124	0.98
TiO ₂ -SPW	0.0136	0.99

Table 7: Kinetic Rate Constants

Statistical Interpretation:

Higher R² values confirm strong kinetic model agreement, validating reproducibility.

The pseudo-first-order kinetic model and statistically significant ANOVA results confirm the reliability and reproducibility of the experimental data, in line with accepted practices in photocatalytic reaction analysis [20].

6.7 Statistical Significance Analysis

A *one-way ANOVA* was applied to degradation efficiencies at 60 minutes.

- F-value: 18.72
- p-value: < 0.001

**Result:**

Differences between pure TiO₂ and agro-waste-modified samples are statistically significant at 99% confidence level.

7. Error and Repeatability Analysis

All experiments were performed in triplicate. Data are presented as mean \pm standard deviation, with relative standard deviation below 5%. The high reproducibility and consistent kinetic trends confirm experimental reliability.

8. Conclusion

This study demonstrates that agro-waste-derived modified TiO₂ photocatalysts can effectively utilize solar energy for passive air purification under Indian AQI conditions. Turmeric and soybean plant wastes emerged as highly effective natural dopants, significantly enhancing visible-light activity, charge carrier separation, and photocatalytic efficiency. The approach offers a sustainable, low-cost, and scalable solution for mitigating air pollution while simultaneously addressing agricultural waste management.

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