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Effect of Cobalt Doped and Cobalt-Yttrium Co-doped TiO_2 Particles Using *Lagenaria siceraria* (Molina) Peel Extract via Green Route for Enhanced Photocatalytic and Antibacterial Performance

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ABSTRACT

The paper displays the synthesis and the overall analysis of pure TiO_2, Co-doped TiO_2 and Co-Y co-doped TiO_2 nanoparticles with a keen focus on their structural attributes, optical, photocatalytic and antibacterial characteristics. The tetragonal anatase phase had been confirmed by X-ray diffraction (XRD) and doping did not induce any secondary phases, but it produced the shifting of the peaks and variation of the intensities. Using the Debye-Scherrer and Williamson-Hall methods to determine crystallite size showed that the size decreases as well as a compressive strain accumulates with the increase of dopants concentration. The UV-Vis spectroscopy revealed that the absorption edge and band-gap narrowing changes at 3.12 eV (pure TiO_2) to 2.80 eV (1% Co -TiO_2) and 2.67 eV (3% Co -Y -TiO_2) and the photo-response extension in the visible regime. The presence of co, Y, and TiO_2 in 3 percent exhibited better results than the pure TiO_2, with 97.48 percent of methylene blue degraded in 120 minutes. Additional antibacterial testing showed that the largest inhibition areas were also at higher concentrations and MIC 25 -40 µg/mL with co-doped samples showing the best activity in Escherichia coli and Staphylococcus aureus. These findings underscore the prospects of Co -Y co-doped TiO_2 as a versatile material in the area of environmental remediation and biomedical uses.

Keywords: Nanoparticles, Anatase, Crystallite, Methylene blue, Antibacterial.

1. Introduction

In recent years, the world has been facing two urgent and interconnected problems: increasing environmental pollution and the rapid spread of harmful microorganisms. Contaminated water bodies filled with organic dyes, industrial effluents, and pathogenic bacteria are becoming common, especially in developing countries. Traditional purification methods like chemical disinfection or filtration often fail to completely remove pollutants, sometimes create toxic by-products, and are not always affordable or sustainable. As deeply concerned citizens about these issues, we wanted to explore a simpler and cleaner solution, sometimes that could degrade pollutants and kill bacteria at the same time, without adding more harmful chemicals to the environment [1], [2], [3].

This is where photocatalysis attracted our attention. Photocatalysis is a light-driven process where a material uses light energy to break down harmful substances. Among the many photocatalysts, TiO_2 (titania) stands out [4], [5], [6]. It is cheap, non-toxic, stable, and already used in everyday products like sunscreens and paints [7]. However, while TiO_2 has great potential, it also has a major weakness: it only works efficiently under ultraviolet (UV) light because of its wide band gap (3.12 eV in the anatase phase) [8]. Since sunlight is mostly visible light, this means TiO_2 cannot use most of the available solar energy. On top of that, even when it absorbs light, it wastes energy before it can do any useful chemical reaction. These two issues, poor visible-light activity and fast charge recombination, are the main reasons why pure titania often shows weak photocatalytic performance [8].

To overcome these problems, researchers around the world have tried many modification strategies: building heterojunctions with other semiconductors, coating them with plasmonic metals, dye sensitization, and so on. But one method stood out to us because of its simplicity and effectiveness, and that is doping [4], [9]. Doping means inserting foreign atoms into the titania lattice to change its electronic structure [10]. Doping can create defective energy levels inside the band gap, which help absorb visible light, and it can trap charge carriers to prevent their recombination [11]. Among various dopants, Cobalt (Co) caught our interest because it has multiple oxidation states (Co^{2+} and Co^{3+}). This means cobalt can introduce new electronic states, promote better light absorption, and even influence the crystal growth and surface activity of TiO_2[9]. Also, cobalt ions can enhance interactions with bacterial cell membranes, which could help kill bacteria more effectively [6], [9]. We also found that rare-earth elements such as Yttrium (Y) can play a very interesting role. Yttrium has a larger ionic radius and strong electronic polarization. When it enters the TiO_2 lattice, it can slightly distort the structure, create oxygen vacancies, and act as an electron scavenger. This can further delay electron-hole recombination and increase the number of active sites on the surface [12].

In this research work, we synthesized three types of TiO_2 particles via the green route: pure, Cobalt-doped, and Cobalt-Yttrium co-doped. We then performed structural,

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morphological, and optical characterizations, followed by tests for photocatalytic dye degradation and antibacterial activity to see how doping and co-doping influence the properties of TiO_2. We aim to show how combining Cobalt and Yttrium doping in green-synthesized TiO_2 can produce low-cost, eco-friendly materials capable of tracking both pollutants and harmful microbes, offering a practical step towards sustainable environmental solutions.

2. Materials and method

2.1 Materials

The following analytical grade chemicals were used without further purification: precursor Titanium (IV) isopropoxide (TTIP, 98%, Merck, India), dopant precursors Cobalt (II) nitrate trihydrate ($Co(NO_3)_2.6H_2O$, 97%, Merck, India), and Yttrium (III) nitrate hexahydrate ($Y(NO_3)_3.6H_2O$, 99.9%, Merck, India). Fresh peels of Lagenaria siceraria (Molina) were used as the green reducing agent. Deionized (DI) water and Ammonium hydroxide (NH_4OH, 25%) were used during synthesis. Methylene Blue was used as the model organic dye for photocatalytic activity evaluation.

2.2 Preparation for Peel Extract and TiO_2 Extraction

All The peels of *L. siceraria* were thoroughly washed with tap water and DI water, then cut into small pieces and oven-dried at 60 °C for 24 h. The dried peels were ground into fine powder. 6.5 g of powder was mixed with 250 mL DI water and stirred at 600 rpm and 60 °C for 1.5 h, followed by ultrasonication at 60 °C for 45 mins. The suspension was filtered, and the filtrate was stored as the peel extract. For pure TiO_2, TTIP was slowly added dropwise into the peel extract (85 mL) under constant stirring (600 rpm) at 80 °C for 3 h until complete hydrolysis. The resulting sol was kept for aging for 24 h to precipitate. Then dried in an oven at 110 °C overnight. Then, the dried sample was crushed into the mortar pestle, and then the sample was taken for the calcination at 450°C for 2 h in an induction furnace to obtain TiO_2 particles. For the doped sample, appropriate molar ratios of cobalt and yttrium precursors (to achieve 1 mol% doping) were co-dissolved with TTIP in the extract under identical conditions, ensuring uniform processing and comparability with the pure sample. The subsequent drying and calcination steps were the same as for the undoped TiO_2

2.3 Characterization of Synthesized TiO_2

The synthesized TiO_2 particles were fully characterized in order to assess their structure, optical, photocatalytic and antibacterial characteristics. Powder X-ray diffraction (XRD) on a Shimadzu LabX XRD-6100 instrument was used to determine the crystal structure, phase composition and purity. The band-gap estimation, optical properties were done with the help of Shimadzu UV-3600 Plus UV-Vis-NIR spectrophotometer. The performance was tested in a controlled condition through UV irradiation of photocatalytic activity in order to evaluate the degradation of the nanoparticles. The minimum inhibitory concentration (MIC) and the antibacterial activity were performed in LB broth medium (Difco Laboratories, India; pH 7.2). To determine MIC, the bacteria samples were inoculated and incubated at 37C° over a period of 24 h, and the minimum concentration of nanoparticles that prevented visible bacteria growth was noted.

3. Result and discussion

3.1 XRD Analysis

Equations To determine the crystal structure of the synthesized pure, Co-doped and Y co-doped TiO_2 nanoparticles, Figure 1a shows the XRD patterns of each of them.

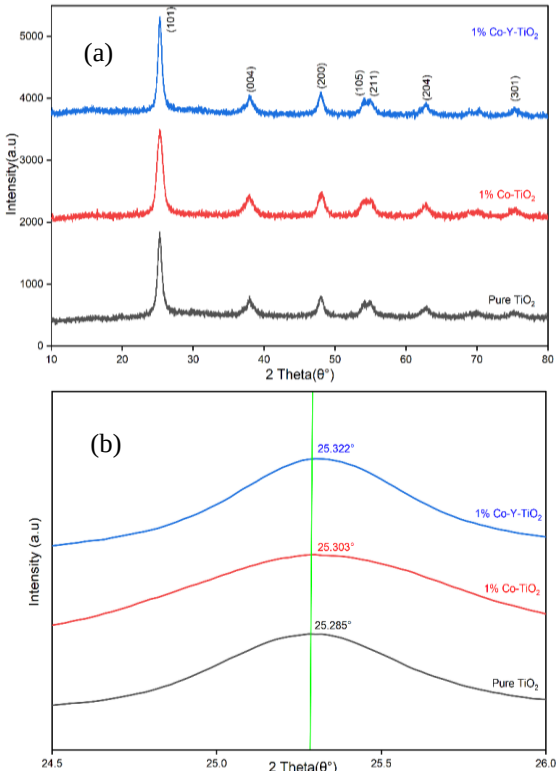

Figure 1. a) XRD Peak position b) Peak shifting after doping and Co-doping

The refinement of samples with the HighScore Plus software indicated that the entire sample crystallized in the tetragonal phase with a JCPDS reference number 00-021-1272 and a space group of I41/amd. At 25.281°, 37.801°, 48.050°, 53.891°, 55.062°, 62.690° and 76.020° the corresponding diffraction peaks of the (101), (004), (200), (105), (211), (204), and (301) planes were observed respectively. Refined lattice parameters were found (a = b = 3.785Å, c = 9.514Å), and unit cell volume (V) was 136.31$Å^3$. No Co or Y dopants diffraction peaks were found and this indicates that the dopants were effectively penetrated into the TiO_2 lattice without forming second phases. Nevertheless, it could be observed that there were minor changes in peak intensity and marginal peak moving, which can be explained by the presence of lattice distortion caused by dopant incorporation.

Table 1. Peak Position, Micro strain and Crystallite Size.

Nanoparticles	**2θ of (101) Peak** ***degree***	**Average Microstrain** ****10^{-3}***	**Crystallite Size** ***nm***	
			Scherrer Size (nm)	Williamson Size (nm)
Undoped TiO_2	25.28	-10.071	9.771	9.592 nm
1% Co-doped TiO_2	25.30	-10.514	9.698	8.992
1% Y-Co co-doped TiO_2	25.32	-10.874	8.931	8.711 nm

The lattice is in compressive strain found by Hall plotting in negative sign [13]. Debye-Scherrer and Williamson-Hall

methods were used to determine the size of the crystallite, macrostrain and density of dislocations and the results are tabulated in [14]

$$D = \frac{K\lambda}{\beta \cos\theta} \quad (1)$$

$$B\cos\theta = \frac{K\lambda}{D} + 4\varepsilon \sin\theta \quad (2)$$

3.2 Uv-Vis Analysis

The optical properties of the synthesized TiO_2 particles were examined using UV-Vis spectroscopy in Figure 2(a-e). Pure TiO_2 exhibited a characteristic absorption peak at 288.55 nm with a bandgap of 3.12 eV. Upon doping, a noticeable red shift in the absorption edge was observed: 1% Co-doped TiO_2 showed a peak at 291.50 nm with a bandgap of 2.80 eV, while 1% Co-Y co-doped TiO_2 shifted to 305.22 nm with a bandgap of 2.67 eV. This trend indicates effective bandgap tuning, with the doping reducing the bandgap and extending light absorption from the UV to the visible region, enhancing potential photocatalytic performance. Bandgap energies were estimated using the Tauc relation [14]

$$\alpha = \frac{A(h\vartheta - E_g)}{h\vartheta} \quad (3)$$

Where α is the absorption coefficient, hν is the photon energy, A is a proportionality constant, and n=2 for direct transitions.

3.3 Photocatalytic Analysis

The Dye degradation of MB indicates a lowering of light absorbance and an increase in particle efficiency, respectively, at various time intervals [15]. Figure *3* shows the absorbance of UV light of the particles of pure, doped, and co-doped materials at 665 nm, where the absorbance peak of the methylene blue solution was found, and the figure represents the decreasing nature in absorbance with increasing time when pure and doped materials samples are used as photocatalysts.

Table 2. UV-Vis bandgap, and Efficiency of doped TiO_2

Nanoparticles	λ_{max} (nm)	Band Gap Energy (eV)	Efficiency (min)				
			0 (min)	30 (min)	60 (min)	90 (min)	120 (min)
Pure TiO_2	288.55 nm	3.12 eV	0	49.16%	56.02%	64.51%	72.85%
1% Co-TiO_2	291.50 nm	2.80 eV	0	37.80%	50.09%	63.18%	77.52%
3% Co-Y-TiO_2	305.22 nm	2.67 eV	0	72.49%	78.04%	85.59%	91.48%

3.4 Antibacterial and MIC Analysis

Figure 4a shows that the synthesized TiO_2 nanoparticles were tested against Gram-positive (Staphylococcus aureus) and Gram-negative (Escherichia coli) strains in terms of antibacterial performance. As controls, TiO_2 nanoparticles and a typical antibiotic (Amoxicillin-30) were used presented on **Figure 5**.

The various concentrations of Punica granatum L. that produced different inhibition zone diameters. The pure and the doped nanoparticles were not found to have any inhibition zones at 100 µg/dish. However, at higher concentration of 200 µg/dish and 400 µg/dish, a significant inhibition effect was recorded with both bacterial strains.

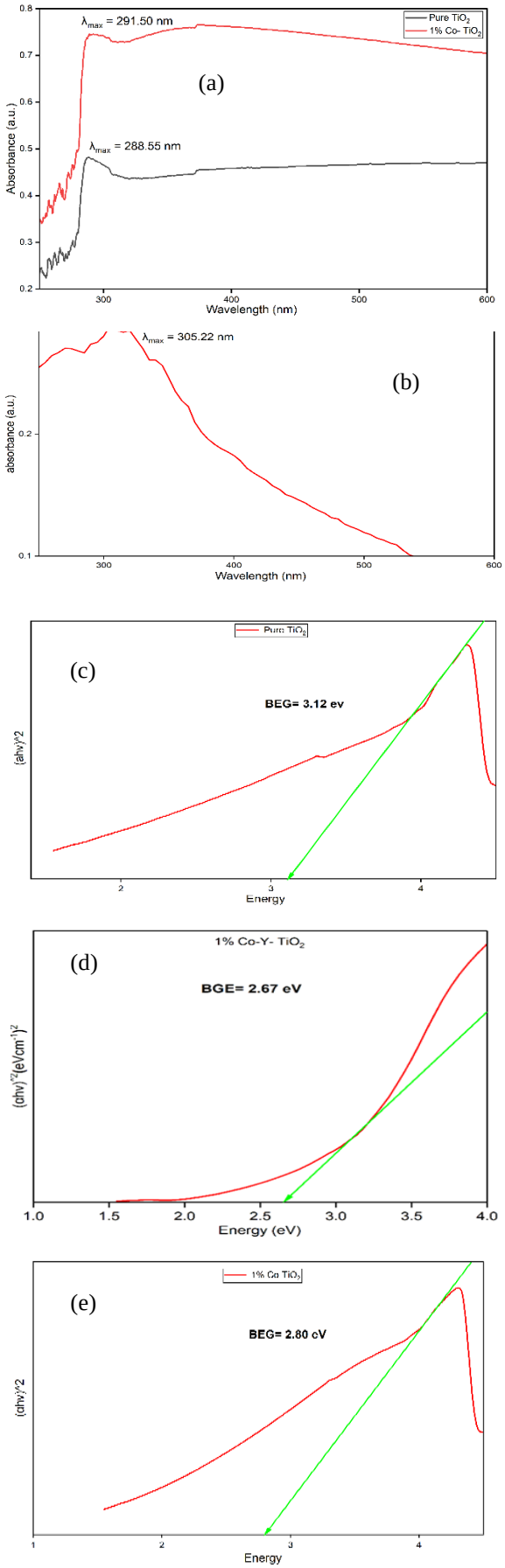

Figure 2. a) λmax of Pure and 1% Co-TiO_2, b) λmax of 1% Co-Y-TiO_2, c) Band gap of Pure, d) 1% Co-TiO2, e) 1% Co-Y-TiO_2

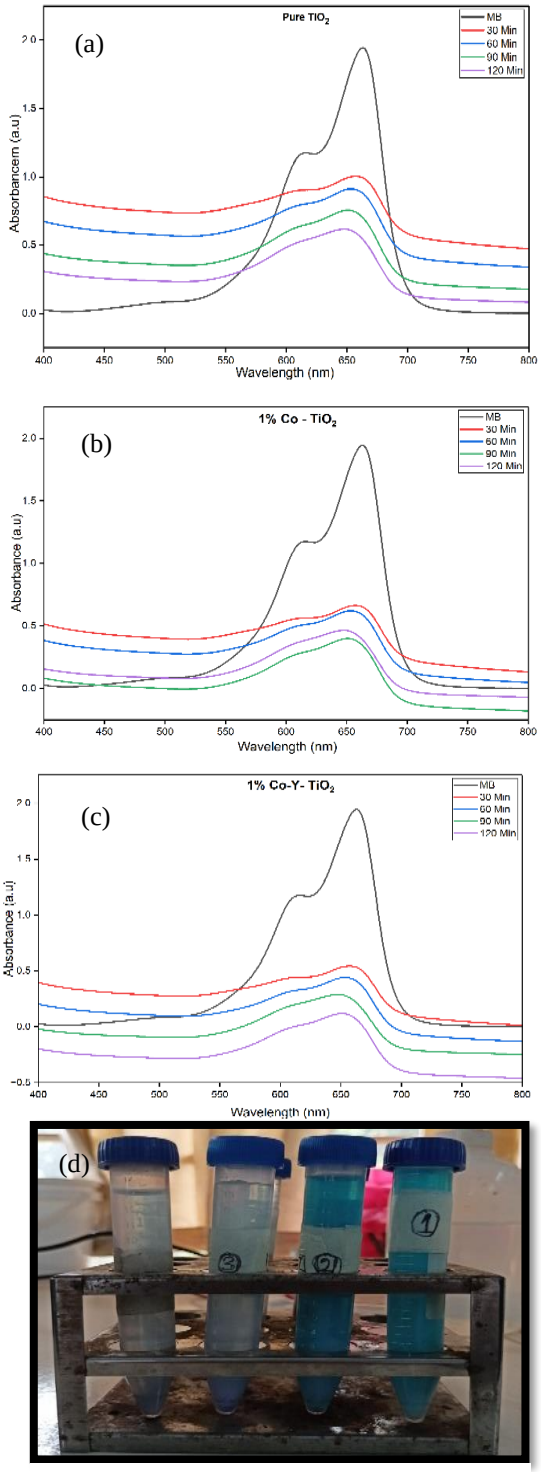

Figure 3. a) UV absorbance of TiO_2, b) 1% Co-TiO_2, c) 1% Co-Y-TiO_2, d) Colour change of MB solution.

Interestingly, the 1% Co–TiO_2 nanoparticles at a concentration of 400 µg/dish had a larger inhibition zone when compared to the standard antibiotic control. On the same note, the 1% Co Y co-doped TiO_2 nanoparticles had a big inhibition zone in the sensitive range, which clearly indicates that it can be used as an effective antibacterial nanoparticle in biomedical tools [16].

The antibacterial efficacy was also confirmed by the establishment of the minimum inhibitory concentration (MIC) values presented on **Figure 4b**. The MIC of pure TiO_2 nanoparticles against S. aureus and E. coli was 25 and 28 ug/mL, respectively.

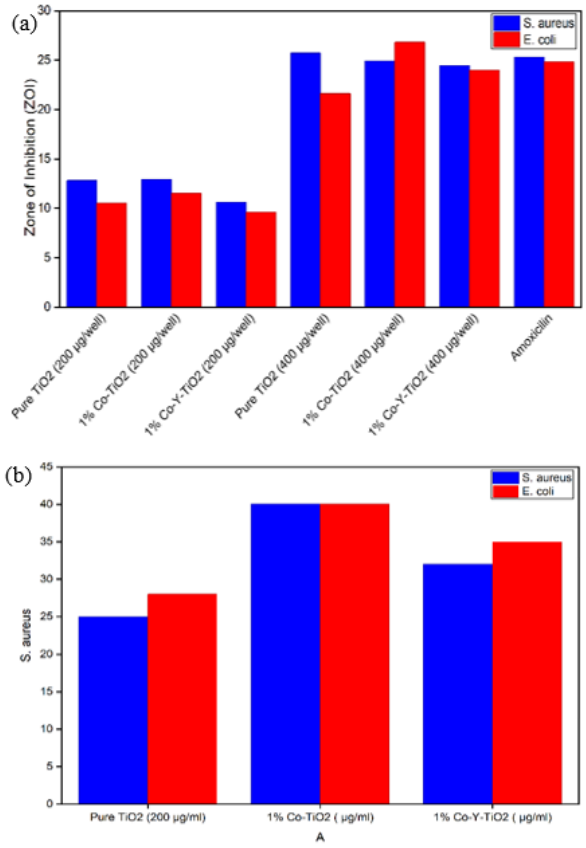

Figure 4. a) Antibacterial Zone of inhibition (ZOI) b) Minimum Inhibition Concentration (MIC)

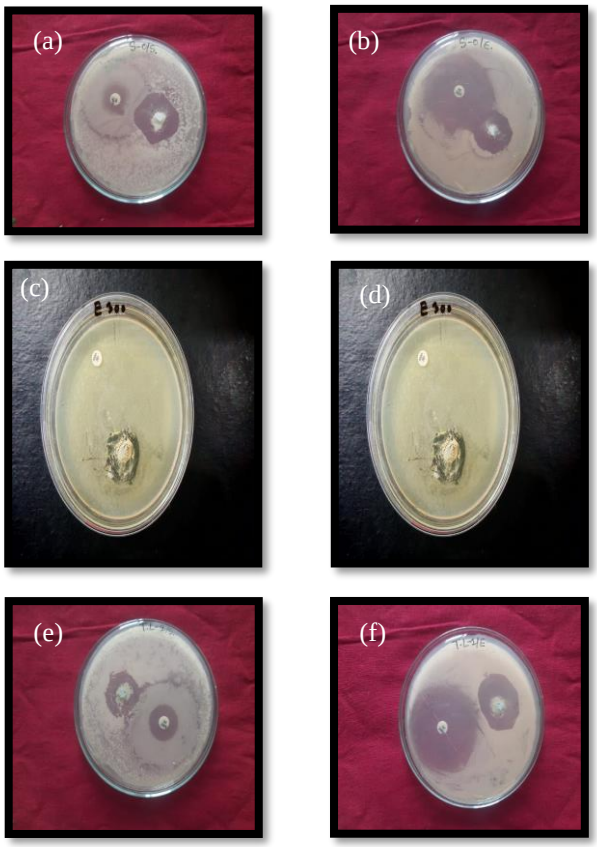

Figure 5. Antibacterial Activities of a), b) Pure, c), d) 1% Co doped, e), f) 1% Co, Y-doped TiO_2 against S. aureus and E.coli Microorganism.

In the case of the 1% Co-TiO_2 sample, the MIC values were 40 ug/mL in both the strains, but with the 1% Co-Y co-doped TiO_2 nanoparticles, the MIC was 32 ug/mL against S. aureus and 35 ug/mL against E. coli. The lowest concentration in which the growth of bacteria was totally suppressed was set as the MIC, which was validated by the lack of turbidity in the culture medium [17]. The reliability of the assay was proven by negative (only medium only) and positive (only medium + bacteria) controls presented on **figure 6**. These results point at the fact that, in spite of the fact that doping affects antibacterial activity, Co and CoY addition to TiO_2 can lead to a significant improvement of the bactericidal activity in higher concentrations, allowing the materials to be considered as good antimicrobial and biomedical candidates.

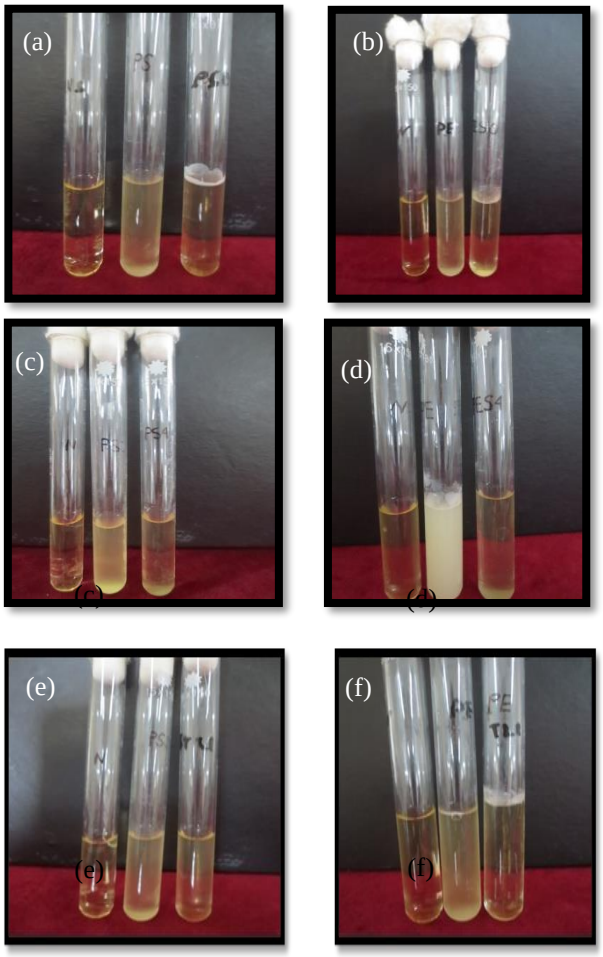

Figure 6. Minimum Inhibition Concentration of a), b) Pure, c), d) 1% Co doped, e), f) 1% Co, Y-doped TiO_2 against S. aureus and E.coli Microorganism.

4. Conclusion

This research work successfully demonstrated the synthesis and comparative evaluation of pure TiO_2, Co-doped TiO_2, and Co-Y co-doped TiO_2 particles, highlighting their enhanced photocatalytic and antibacterial properties. UV-Vis analysis revealed a progressive red shift in absorption edge accompanied by a bandgap narrowing from 3.12 eV (pure) to 2.80 eV (1% Co-doped) and 2.67 eV (3% Co-Y co-doped), effectively extending photo-response from the UV into the visible region. This bandgap tuning translated into markedly improved photocatalytic degradation efficiencies, with 3% Co-Y co-doped TiO_2 achieving 97.48% degradation of methylene blue within 120 mins, compared to 72.85% for pure TiO_2. Beyond photocatalysis, the co-doped particles exhibited notable antibacterial activity against Escherichia coli and Staphylococcus aureus, with clear inhibition zones at higher doses and an MIC of 40 µg/mL for strains. These findings demonstrate that strategic co-doping can synergistically improve the optoelectronic and biological performance of TiO_2, making it a promising multifunctional material for environmental remediation and antimicrobial applications.

5. Acknowledgement

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