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Cu-doped C₃N₄-MgO nanorods for bactericidal and dye degradation performance

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Full Title:	Cu-doped C ₃ N ₄ -MgO nanorods for bactericidal and dye degradation performance
Article Type:	Original Article
Abstract:	<p>Photocatalytic and magnetic stability of two-dimensional layered nanomaterials is improved by metal doping, which is a potential eco-friendly technique widely used in various industrial sectors. In this study, economical and convenient co-precipitation method was adopted to synthesize copper (Cu) doped in various concentrations (2.5, 5, 7.5 and 10%) into fixed amount of C₃N₄/MgO nanostructures for efficient photocatalytic and bactericidal activities. Improved crystallinity and increase in crystal size upon doping was confirmed with XRD analysis, which was corroborated with SAED results. FTIR spectroscopy revealed that MgO spectra consisted of stretching vibrations of Mg-O bond and other functional groups with minor changes in the vibrational modes upon doping. A HR-TEM fitted with Gatan® digital software indicated the formation of hexagonal phase in as-prepared sample and nanorods upon doping, with confirmed d-spacing values. The UV-Vis analysis revealed a slight redshift in absorption intensity leading to decreased band gap (E_g) for Cu-doped MgO/C₃N₄. Photoluminescence (PL) spectra were acquired to investigate the recombination of electron-hole pairs. To evaluate the elemental and surface composition with binding energy alterations of Cu-doped C₃N₄-MgO nanorods, XPS was employed. Thermal stability and behavior of synthesized samples was investigated by DSC thermoanalytical analysis. Photocatalytic performances of as-prepared samples were evaluated against methylene blue ciprofloxacin (MBCF) dye in acidic, neutral and basic medium. Furthermore, efficient antibacterial potential was evaluated against Escherichia Coli (E. coli) and Staphylococcus aureus (S. aureus) bacteria.</p>

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4 **Cu-doped C₃N₄-MgO nanorods for bactericidal and dye degradation performance**
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4 **ABSTRACT**
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7 Photocatalytic and magnetic stability of two-dimensional layered nanomaterials is improved by
8 metal doping, which is a potential eco-friendly technique widely used in various industrial
9 sectors. In this study, economical and convenient co-precipitation method was adopted to
10 synthesize copper (Cu) doped in various concentrations (2.5, 5, 7.5 and 10%) into fixed amount
11 of C₃N₄/MgO nanostructures for efficient photocatalytic and bactericidal activities. Improved
12 crystallinity and increase in crystal size upon doping was confirmed with XRD analysis, which
13 was corroborated with SAED results. FTIR spectroscopy revealed that MgO spectra consisted of
14 stretching vibrations of Mg-O bond and other functional groups with minor changes in the
15 vibrational modes upon doping. A HR-TEM fitted with Gatan® digital software indicated the
16 formation of hexagonal phase in as-prepared sample and nanorods upon doping, with confirmed
17 d-spacing values. The UV-Vis analysis revealed a slight redshift in absorption intensity leading
18 to decreased band gap (E_g) for Cu-doped MgO/C₃N₄. Photoluminescence (PL) spectra were
19 acquired to investigate the recombination of electron-hole pairs. To evaluate the elemental and
20 surface composition with binding energy alterations of Cu-doped C₃N₄-MgO nanorods, XPS was
21 employed. Thermal stability and behavior of synthesized samples was investigated by DSC
22 thermoanalytical analysis. Photocatalytic performances of as-prepared samples were evaluated
23 against methylene blue ciprofloxacin (MBCF) dye in acidic, neutral and basic medium.
24 Furthermore, efficient antibacterial potential was evaluated against Escherichia Coli (*E. coli*) and
25 Staphylococcus aureus (*S. aureus*) bacteria.
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54 **Keywords:** Co-precipitation, C₃N₄, nanorods; MgO; Antimicrobial; XPS; DSC-TGA
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4 **1. INTRODUCTION**
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7 Nanotechnology has evolved into a fascinating discipline in the current period, with several
8 applications in biology, health, energy, and materials science, among others [1–5].
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10 Approximately, 5-10 billion dollars per year are being spent on clinical complications associated
11 with infected implanted medical devices that prolong hospital stays and cause medical
12 complications for patients [6]. Typical antibiotics used to treat nosocomial infections are not able
13 to penetrate biofilms, which results in making bacteria and fungi more drug resistant and hard to
14 eliminate. [7, 8]. Therefore, biomaterials are crucial to eliminate microbial infections and
15 linkage, reducing antibiotics use and extenuating infections of medical devices [9].
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19 Many metal oxide nanoparticles (NPs) have been used for this purpose as they have shown
20 considerable antimicrobial properties. Metal-oxide NPs are extremely fascinating due to their
21 remarkable applications in the electronics fields, catalysis, sensing, and so forth [10–19].
22
23 Fabrication of metal oxide NPs with different morphologies is becoming prominent due to their
24 significant properties [20, 21]. High surface-to-volume ratio of one-dimensional nanostructures
25 including wires, fibers and rods make them highly attractive for various applications [22]. From
26 among all metal oxides, MgO (magnesium oxide) is a potential oxide that can be prepared easily
27 in versatile structural forms and different sizes [23]. MgO has found many applications in the
28 field of photocatalysis, bio-compatibility and antibacterial activities. MgO NPs have been used
29 as substantial material in bioremediation, additives in refractories, superconducting products,
30 water treatments, paints and specially in medicines for the relief of heartburn, sore stomach, acid
31 digestive disorders and for bone regeneration [24–26]. This is due to the wide energy band gap
32 E_g , thermochemical stability and impressive surface reactivity of MgO NPs [27]. Various
33 precursors have been utilized for MgO preparation using different methods co-precipitation, sol-
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4 gel, combustion, hydrothermal and spray pyrolysis [13, 28, 29]. Different crystal structures can
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6 be obtained from metal elements of different oxides which can be insulators, semiconductors and
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8 metallic, that are very useful in chemical reactivity [30]. In principle, behavior of metal
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10 containing molecules in different oxides depend on electrostatic force produced by charges and
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12 mixing of orbitals of molecules with conduction and valance bands (CB and VB respectively),
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14 and dipole of molecules [31].
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19 Due to physiochemical nature of metal-containing elements exhibiting some interesting
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21 properties such as large E_g , chemical inertness, thermal stability and high dielectric constant,
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23 MgO has become one of the most important materials in industry today [32, 33]. MgO as a bulk
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25 material have a very large E_g which reduces its application as a semiconductor [34]. Doping of
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27 metals in metal oxides tend to decrease E_g of materials normally making them conductors and
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29 advances its applications in electronics. Cu is a very interesting metal as it contains negatively
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31 charged electron in its complete orbital near positive charged nucleus. Application of Cu is very
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33 fascinating in antibacterial activity, as very low amount of Cu induces inactivation of bacteria in
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35 dark [35]. This enhanced antibacterial effect is mainly attributed to Cu ions, surface contact
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37 killing and Cu obtaining reactive oxygen species (ROS) in O_2 presence. This bacterial
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39 inactivation by Cu has been recorded to take place in both anaerobic and aerobic conditions [36].
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41 Graphitic carbon nitride (C_3N_4) is also an interesting compound for its application in
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43 photocatalysis and antimicrobial activities. In several carbon compounds, C_3N_4 surface offers
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45 electron rich qualities and multiple modified functionalities. Water decomposition by C_3N_4 is a
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47 milestone when it comes to its application in photocatalysis. This is ascribed to the fact that this
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49 novel material does not contain metal and metallic elements and causes unnecessary damage and
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51 environmental toxicity [37]. Aim of this study is to prepare Cu-doped C_3N_4 /MgO nanostructures
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4 with various Cu concentrations, via co-precipitation method and to check its antimicrobial and
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6 photocatalytic properties.
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8 9 10 **2. EXPERIMENTAL DETAILS**

11 12 13 **2.1 Materials**

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16 Magnesium chloride ($\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$, 99-102%), copper chloride ($\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$, 99%) and urea
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18 ($\text{CH}_4\text{N}_2\text{O}$) were obtained from Sigma Aldrich, Germany. Carbon nitride ($\text{g-C}_3\text{N}_4$) was obtained
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20 via pyrolysis of urea ($\text{CH}_4\text{N}_2\text{O}$). Without further purification, all chemicals have been utilised.
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23 24 **2.2 Synthesis of MgO and Cu-C₃N₄/MgO**

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27 Controlled material (MgO) was prepared in laboratory. Briefly, $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ (4g) was dissolved
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29 in 100 mL of deionized (DI) water and the mixture was allowed to react for 15 min under
30
31 constant stirring. One molar solution was prepared in 100 ml of water with 4g of ($\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$)
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33 and 100 mg of (C_3N_4) was added in solution (Fig. 1). Firstly, solution of ($\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$) and
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35 (C_3N_4) was prepared and then different concentrations (2.5%, 5%, 7.5% and 10%) of
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37 ($\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$) were doped into solution of $\text{C}_3\text{N}_4/\text{MgO}$. Firstly, prepared solution was put on hot
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39 plate at 200°C for three hours under constant stirring. Following this, sample was sonicated for
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41 half an hour with ultrasonic rays followed by centrifugation at 7500 rpm for ten min. Lastly,
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43 samples were annealed at 450°C for two hours.
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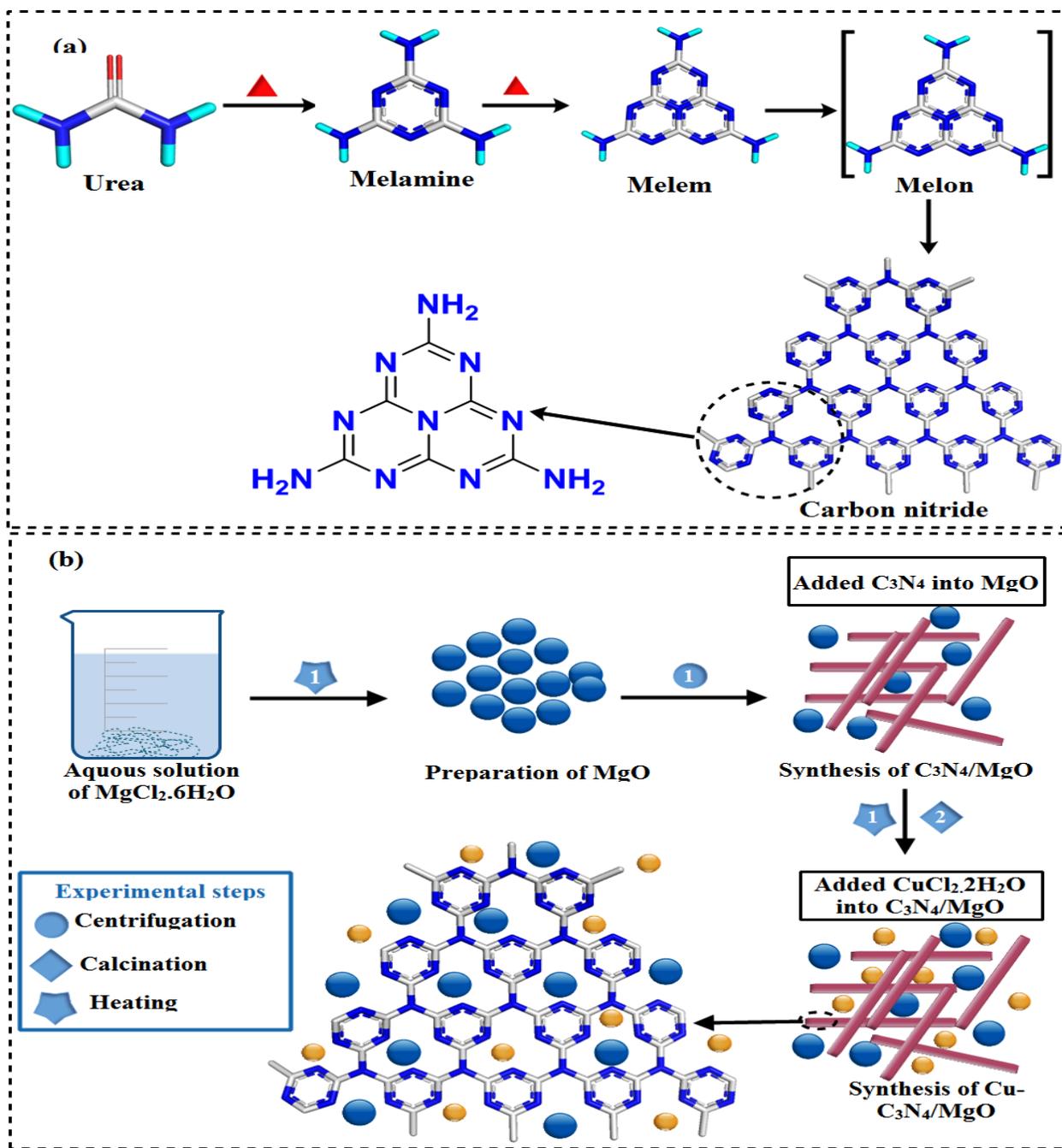


Figure. 1 (a) Formation mechanism of carbon nitride obtained from urea pyrolysis. (b) Schematic illustration of fabrication of $\text{Cu-C}_3\text{N}_4/\text{MgO}$ samples.

3. RESULTS AND DISCUSSION

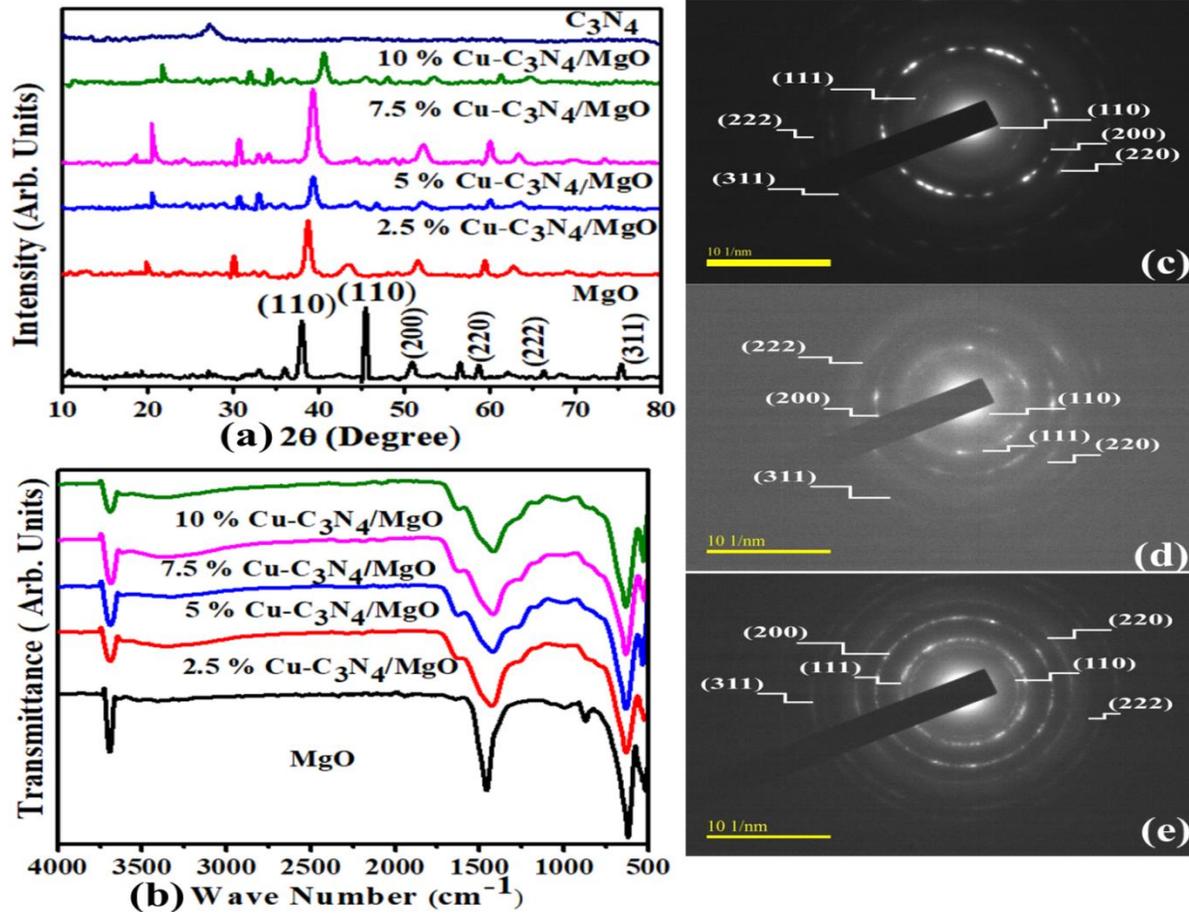


Figure 2. (a) XRD spectra (b) FTIR spectra and SAED patterns of MgO (c), 7.5% Cu- C_3N_4 /MgO (d) and 10% Cu- C_3N_4 /MgO (e).

Structural and phase properties of prepared samples were examined through x-ray diffraction in 2θ range 8° - 80° as depicted in **Fig. 2 (a)**. Peaks generated at 38.01° , 45.03° , 50.87° , 58.67° , 66.17° and 76.53° indexed to (110), (111), (200), (222), (220), and (311) planes, respectively belonged to FCC cubic structure of MgO (JCPDS Card No. 87-0653). C_3N_4 peaks were not detected in doped samples due to their lower concentration relative to MgO. The impact of

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4 dopants Cu and C₃N₄ were found in peaks shift toward higher 2θ° values. Upon doping, peak
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6 broadening was observed which led to decrement in crystalline size and showed successful
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8 incorporation of dopants into the matrix [38]. Peaks (200), (220) and (311) contracted for doped
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10 samples might indicate distortion of typical FCC crystalline structure at least in some specific
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12 directions identifying rod-like structure of prepared samples. Additional peaks observed at
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14 33.03°, 51.09° and 56.87 in spectra depicted the presence of hydroxyl group Mg(OH)₂ [39]. Fig
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16 2(c-e) shows SAED (Selected Area Electron Diffraction) patterns for MgO,7.5% and 10% Cu-
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18 doped C₃N₄MgO indexed with planes (110), (111), (200), (220), (222) and (311) of MgO that
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20 were compatible with XRD results. To analyze chemical composition and the presence of
21
22 various functional groups in samples, FTIR spectroscopy was performed (Fig. 2b). The broad
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24 band range (3040–3550 cm⁻¹) indicated MgO nanostructures formation while broad band in 620-
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26 873 cm⁻¹ range was ascribed to vibrations of Mg-O bond [25, 40]. The distinct bands observed at
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28 880 and 1410 cm⁻¹ represent vibrations of surface hydroxyl group (1). Sharp peak at 3695 cm⁻¹ is
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30 accredited to stretching of O–H bond.
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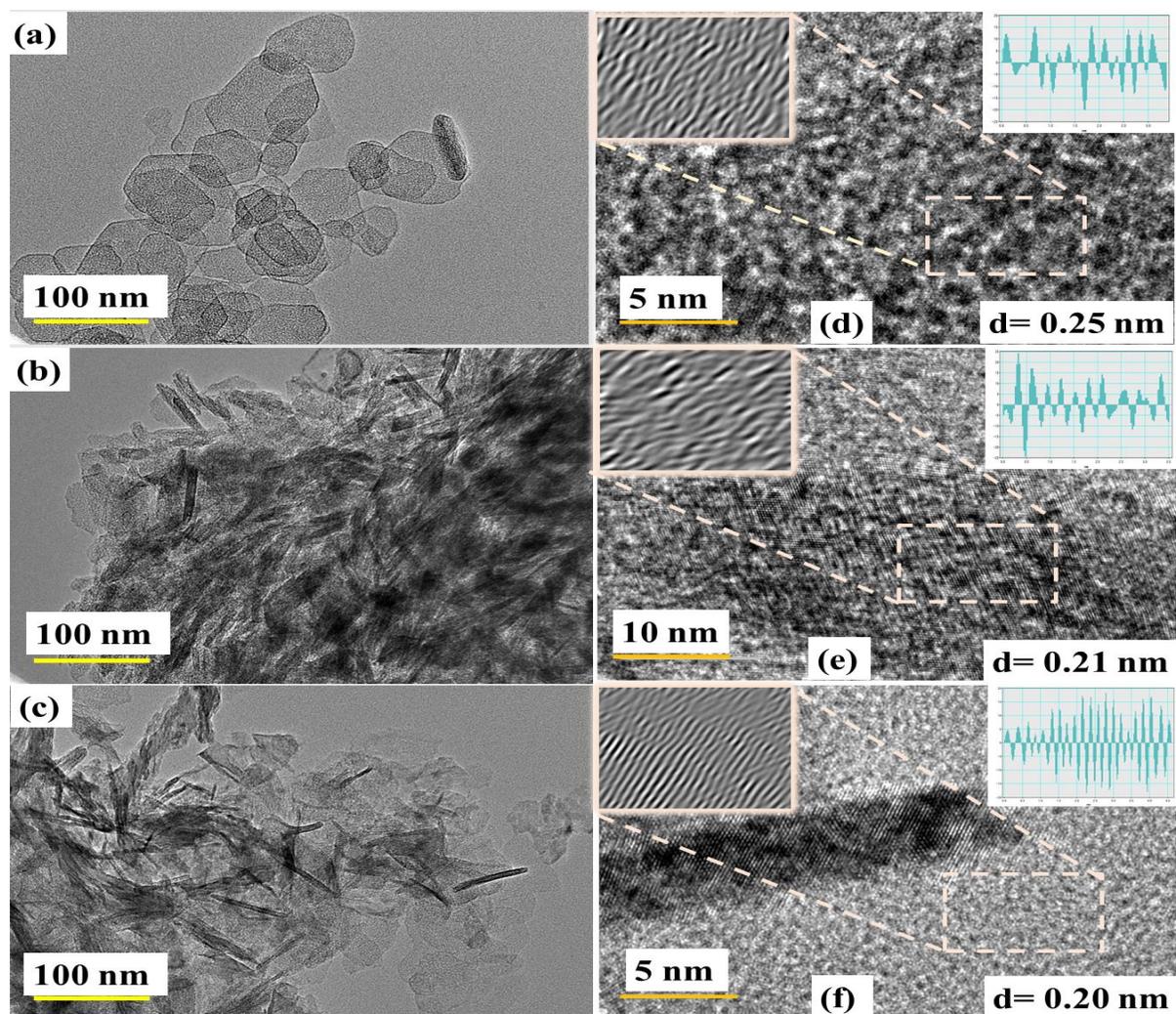


Figure 3: (a) MgO (b) 7.5% and (c) 10% Cu-C₃N₄/MgO illustrated HRTEM images and lattice fringes of MgO, 7.5% Cu-C₃N₄/MgO and 10% Cu-C₃N₄/MgO are represented in (d), (e) and (f), respectively.

HRTEM was employed to study the morphology and surface topology of prepared samples. Image of 100 nm size for MgO exhibited cubic structure formation due to the aggregation of several thousand NPs (Fig. 3a). 7.5% and 10% Cu-doped C₃N₄/MgO depicted dense and interconnected nanorods such that no clear boundary existed between them, see (Fig. 3b) and (Fig. 3c) respectively. Lattice fringes were separated by distance of 0.25 nm, 0.21 nm and 0.20

nm for MgO, 7.5% Cu-C₃N₄/MgO and 10% Cu-C₃N₄/MgO, respectively (Fig. 3(c-e)). HRTEM and d-spacing of 2.5 and 5% samples are shown in Fig. S1.

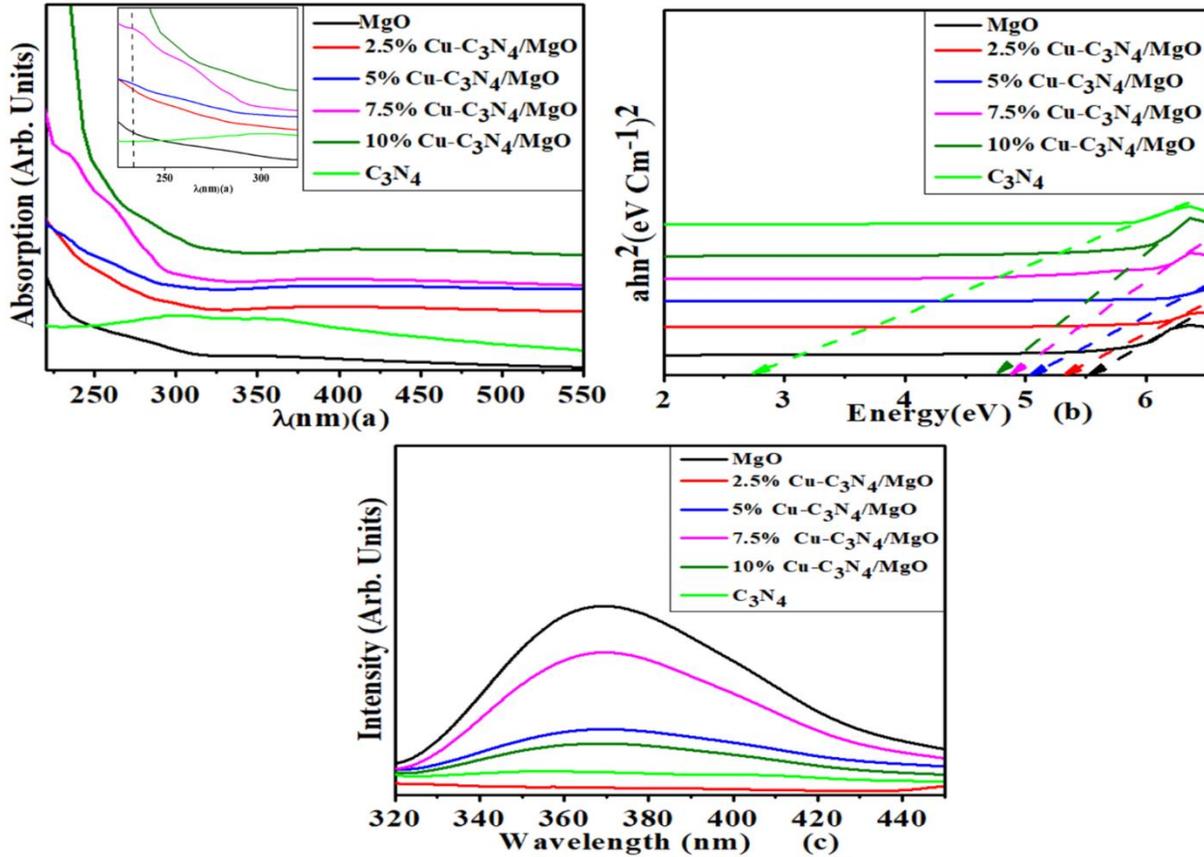


Figure 4: (a) Band gap (b) UV-Vis Spectra (c) PL spectra of prepared samples.

The optical absorption spectra of MgO- and Cu-doped C₃N₄/MgO were recorded to investigate typical properties in UV-Vis region (Fig. 4a). MgO showed absorption in the region 230-310 nm and redshift was observed upon increasing concentration of Cu in C₃N₄/MgO composites. This absorption is significantly greater than bulk MgO because of bulk excitonic transitions. This is due to the electrostatic potential of O₂ in MgO which slowly decreases with coordination and the whole process requires lesser energy [41]. Quantum confinement upon impurity incorporation is

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4 dependent on host crystal size, as crystal size decreases confinement degree and its effect
5 increases [38]. The optical E_g of obtained samples were calculated from the Tauc's relation as
6 represented in Fig. 4b. E_g for MgO was calculated to be 5.5 eV and it decreased down to 4.7 eV
7 for Cu-doped C_3N_4/MgO . This decrease in E_g is ascribed to smaller crystallite size and
8 agglomeration of particles to form nanorods upon doping [32].
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17 When light falls on the surface of a material, generation of electron-hole pairs and their
18 recombination lead to PL phenomenon. PL spectra for prepared samples are shown in Fig. 4c.
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20 Emission spectra depicted one dominant peak at 370 nm, with excitation wavelength 280 nm
21 irradiated onto the samples. MgO being an insulator ($E_g \sim 5.7$ eV) showed luminescence in the
22 above-mentioned range, which is extensively ascribed to surface defects and vacancy sites
23 excitations [42]. Photo-excitation of electrons into CB of attached oxygen atoms at step-edge
24 defects of MgO causes luminescence [43]. Spectra recorded for Cu-doped C_3N_4/MgO composite
25 showed significant decrease in PL intensity which may be attributed to increased amount of
26 surface and structural defects generated after incorporation of Cu atoms in the matrix. This
27 dramatic increase in defects act as trap sites for electrons, rendering their motion toward holes
28 thus reducing recombination rate of excitons.
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46 Differential scanning calorimetry (DSC) was utilized to measure the flow of heat into or out of
47 the samples (MgO, 5% Cu- C_3N_4/MgO and 10% Cu- C_3N_4/MgO) as a function of temperature and
48 heat flow. The DSC curves exhibited a distinctive endothermic peak at 144 °C for pure MgO and
49 this peak started to shift forward upon Cu and C_3N_4 doping into the matrix, as presented in Fig.5.
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51 For 5% Cu- C_3N_4/MgO , data showed an endothermic peak at 154 °C and for 10% Cu- C_3N_4/MgO
52 the endothermic peak is at 185 °C. This shift of endothermic temperature region towards higher
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4 temperature range might be attributed to the increasing concentration of Cu in C₃N₄/MgO
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6 sample, as Cu exhibits an endothermic peak at a higher temperature region (300-450 °C) [44].
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9 These distinctive peaks indicate the purity and thermal stability of the prepared samples [45–47].
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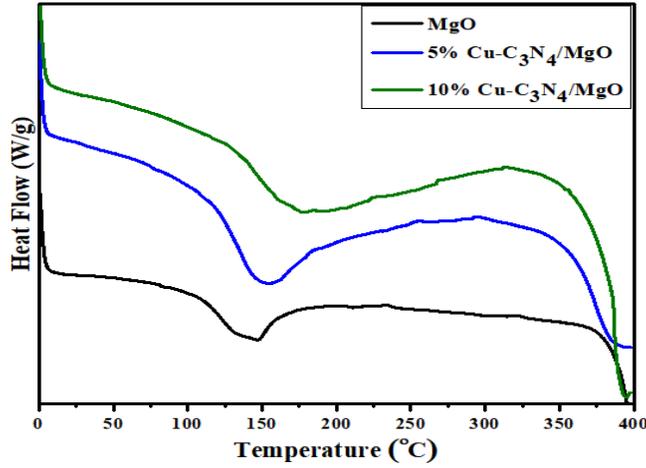


Figure 5. DSC spectra of MgO, 5% Cu-C₃N₄/MgO and 10% Cu-C₃N₄/MgO.

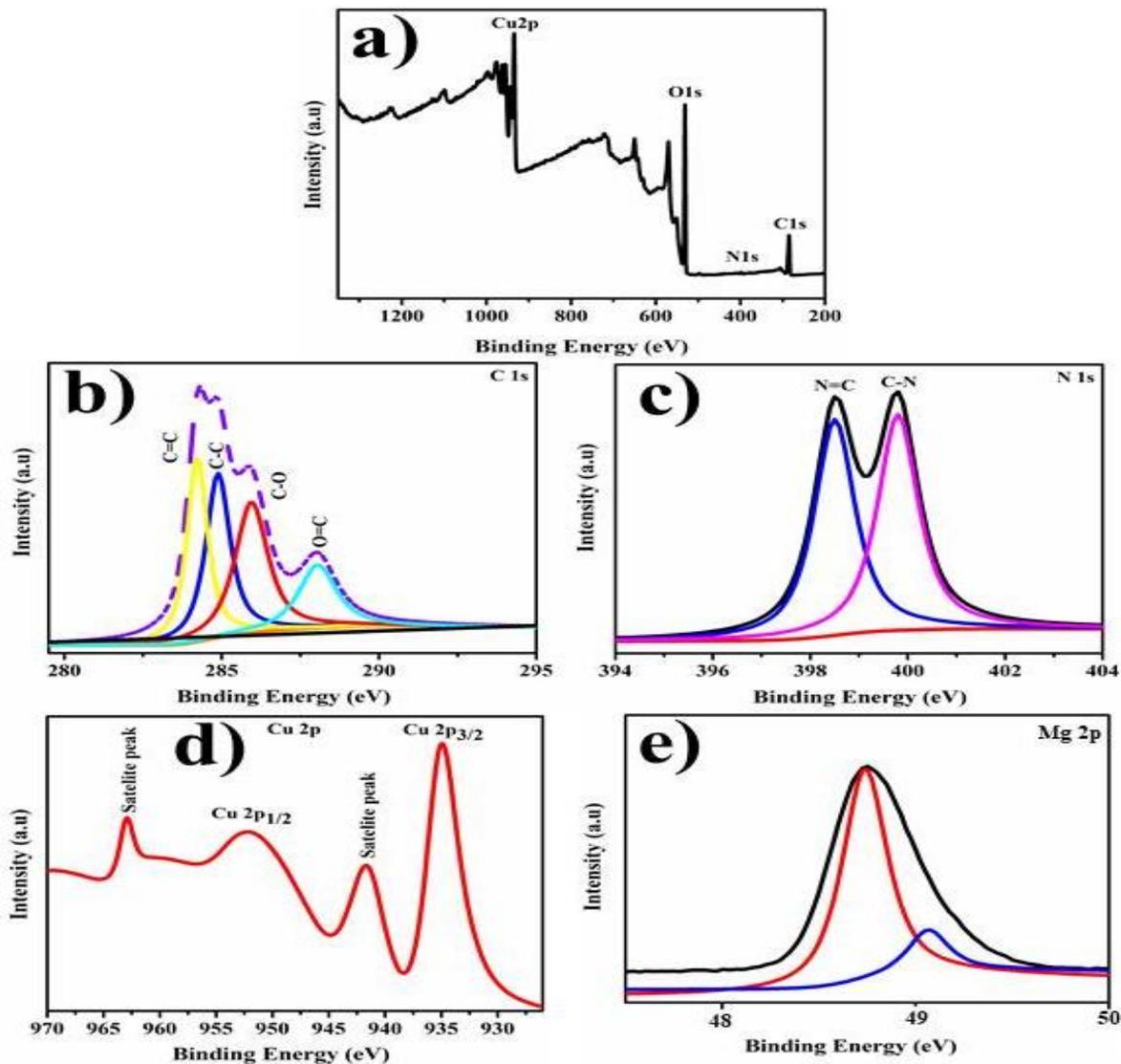


Figure 6: XPS spectra of Cu-doped C_3N_4/MgO samples.

The elemental composition, surface composition, and binding energy alterations of Cu-doped C_3N_4-MgO nanorods were determined using XPS. The survey, O 1s, N 1s, and Cu 2p high resolution spectra are shown in Fig. 6(a-e). The XPS survey spectrum displays the predicted strong signals of C, N, O, and Cu, as seen in Fig. 6 (a). The C1s peaks of the doped nanorods may be resolved into three peaks at 284.8, 286.4, and 288.4 eV, referring to the functional groups C-C/C=C, C-O, and C=O, accordingly as depicted in Fig. 6b [48]. Moreover, the N1s signal band in Fig. 6 (c) may be attributed to the N=C and C-N groups due to its binding energy of

around 398.5 and 399.8 eV [49]. Notably, Fig. 6 d defined the Cu 2p pattern of doped CuO with heights at 933.3 and 953.3 eV binding energies, which correspond to the Cu 2p_{3/2} and Cu 2p_{1/2} spin orbits, accordingly, confirming the samples' divalent oxidation state. The last two peaks, at 942.2 and 962 eV, relate to the satellite heights of Cu 2p_{3/2} and Cu 2p_{1/2}, which emerged principally owing to the partially filled 3d⁹ orbital in divalent oxidation state [50]. A high-resolution analysis of the Mg 2p core level spectrum reveals two distinct electronic states (2p_{1/2}, 2p_{3/2}) with binding energies of 48.95 eV and 49.29 eV, respectively. The location of the 2p_{3/2}, 2p_{1/2} peaks and the difference in their binding energies indicate the presence of Mg ions in the +2 oxidation state as shown in Fig. 6 (e) [51].

Table 1: Bactericidal action of MgO and Cu-doped C₃N₄/MgO

Pathogen	0.5mg/50μl					1.0mg/50μl				
	1	2	3	4	5	1	2	3	4	5
S. aureus	1.55	2.65	3.45	3.95	4.05	2.05	4.4	5.35	6.45	7.05
E. coli	1.45	2.6	3.3	3.65	3.95	1.8	3.15	3.4	3.85	5.15

¹ MgO

² 2.5% Cu-C₃N₄/MgO

³ 5 % Cu-C₃N₄/MgO

⁴ 7.5% Cu-C₃N₄/MgO

⁵ 10% Cu-C₃N₄/MgO

Fig. S2 shows the photo-degradation of methylene blue ciprofloxacin (MBCF) dye over MgO and Cu-C₃N₄/MgO nanorods as catalyst. The dye degradation in photocatalytic procedure is

caused by generation of electron-hole (e^-h^+) pairs in VB and CB. Produced h^+ in VB reacts with surrounding water molecules to form OH^\bullet radicals and e^- in the CB is captured by the oxygen to generate anionic superoxide radical ($O_2^{\bullet-}$) as illustrated in Fig. 7 and explained in following equations [52]:

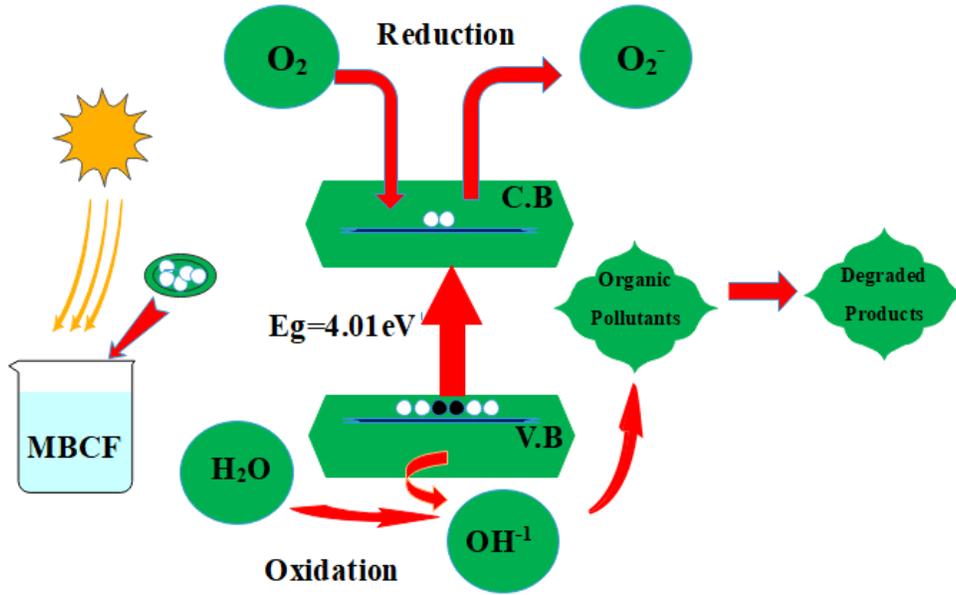
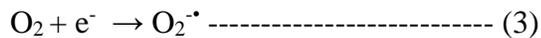


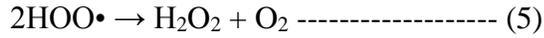
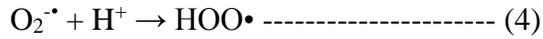
Figure 7. Illustrates photocatalytic mechanism of Cu-C₃N₄/MgO samples.



The generated $\bullet OH$ radical are remarkably strong oxidizing agents. Molecules adsorbed or near to the surface of the catalyst are non-selectively attacked by $\bullet OH$ radical species which result in degradation or mineralization based on structure and stability level. The electrons in the VB interacts with oxygen molecules to generate $O_2^{\bullet-}$ species as shown in equation 3,



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4 This produced superoxide gets protonated and form a hydroperoxyl radical (HO₂•) and further
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6 dissociates into highly reactive hydroxyl radicals (OH•) as presented in below equations,
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19 The E_g of MgO is 7.8 eV normally, but for MgO nanostructures this is decreased to 5.5 eV which
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21 makes it a potential material for photo-catalysis [53, 54].
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24 Percentage degradation of individual material is calculated using equation 7 as shown in Fig. 8
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26 [40]:
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29 $\% \text{ Degradation} = \left(\frac{C_o - C_t}{C_o} \right) * 100$ ----- (7)
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32 Here C_o and C_t are the initial and final concentration of dye after exposure to UV-Vis light.
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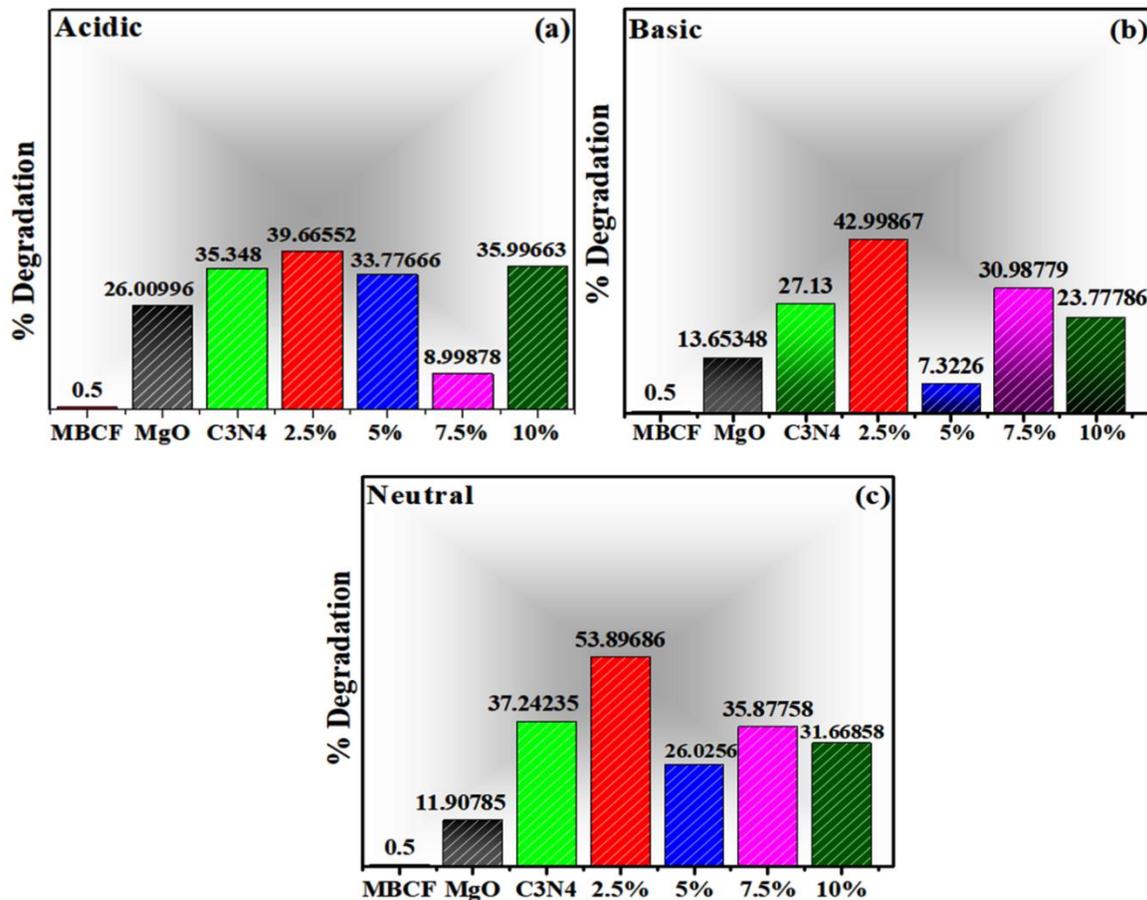


Figure 8: Representing the photocatalytic degradation percentage of samples in acidic, basic and neutral solution of MBCF dye.

The degradation % is minimum for the samples when dye is placed in the dark. Fig. 8 indicated that MBCF dye degradation percentage is maximum (53.89%, 42.99% and 39.66%) for 2.5% Cu-C₃N₄/MgO in neutral, basic and acidic solutions of MBCF dye, respectively. The decrease in degradation on further increasing the doping concentration shows that these nanostructures are the best performing catalyst with 2.5% doping of Cu in C₃N₄/MgO. As described earlier in XRD section, crystallite size decreased with increasing amount of dopants. Addition of Cu (2.5 %) into C₃N₄/MgO showed maximum degradation performance as confirmed by PL results. The 2.5 % sample showed minimum recombination rate which might be owed to the increased amount of

defects produced in the lattice after doping [34, 55]. Moreover, the smaller crystallite size reduces the recombination rate and more particles (electrons and holes) are transferred to the surface of catalysts. Cu-doping in C_3N_4/MgO may be due to the balance of trapping carriers causing the longer lifetime of surface charge carriers which results in enhancing PCA [25, 56]. The role of C_3N_4 in fixed amount is very crucial for dye degradation as well. C_3N_4 -doped into MgO tend to increase the absorption ability of the sample with an increase in pH and then it starts decreasing [57].

The degradation percentage for the neutral solution of MBCF was maximum, which ascribed to the balancing of hydroxyl groups and holes at the surface. The lower percentage degradation for acidic solution may be due to the fact that dye decomposition takes place at catalyst surface and hydroxyl ions deficiency to react with holes to produce hydroxyl radicals [25]. For basic solution, the degradation percentage of dye decreases, which may be due to the decrease of positive charge at photo-catalyst surface because OH^- ions are absorbed into it [58–60]. A comparison between $Cu-C_3N_4/MgO$ and other famous photocatalysts is provided in the Table 2.

Table 2: Presents the comparison between several famous photocatalysts for the degradation of MB and some other dyes.

Materials	Dyes	Degradation (%)	Time (min)	References
TiO_2	MB	86	120	[61]
V- TiO_2	MB	45	1	[62]
$Fe_3O_4/TiO_2/Ag$	MB	90	100	[63]
$Fe_3O_4@ZnO$	MBCF	86	240	[64]

g-C ₃ N ₄	RhB	20	100	[65]
g-C ₃ N ₄ in NaOH	Aqueous Cr ⁺	29.4	120	[66]
Cu-C ₃ N ₄ /MgO	MBCF	53	80	Present study

The photo-degradation kinetics by determining the slopes on $\ln\left(\frac{C_t}{C_0}\right)$ curves were drawn versus time (Fig. 9). The rate constants (k) of all samples were determined by pseudo 1st order kinetic equation, $\ln\left(\frac{C_0}{C_t}\right) = kt$

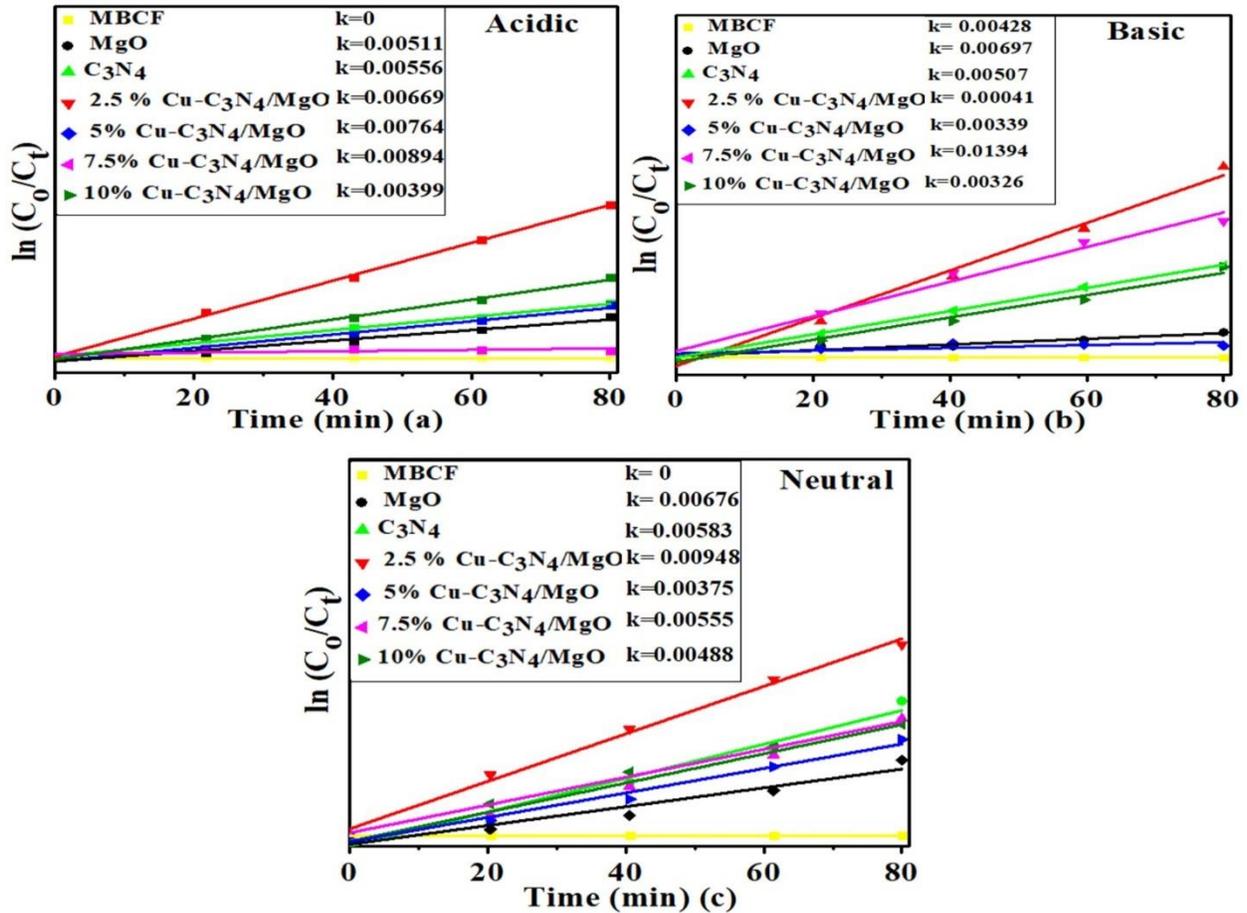


Figure 9: $\ln(C_0/C_t)$ vs time graph of prepared samples at (a) acidic, (b) basic and (c) neutral nature.

Disc diffusion technique was utilized to screen bactericidal sensitivity of prepared nanocomposites. Inhibition zones measured for prepared samples ranged from 1.45 mm to 7.05 mm in diameter against G-negative and positive [Table. 3]. The maximum zone of inhibition observed for 10% Cu- C_3N_4 /MgO against *S. aureus* and *E. Coli* were 7.05 mm and 4.15 mm, respectively. Other samples showed comparatively less bactericidal potential which is ascribed to low concentration (0.5 mg/50 μ l) as only few NPs are available to cooperate with cell wall. Overall, bactericidal performance of prepared products is better against *S. aureus* at both high and low concentration. Previous studies have reported that bactericidal performance of MgO

nanocomposites depends upon the size. This activity increases slowly by decreasing MgO particle size in the range ~ 45-70 nm [67]. This enhanced performance of C₃N₄/MgO with maximum doping of Cu (10%) may be due to incorporation of dopant into matrix which tends to decrease the E_g and crystallite size of the prepared sample. This improved performance can be ascribed to the interaction of microbe cell membranes (having negative charge) and Cu²⁺ and Mg⁺² ions released by doping with Cu. Released positive ions penetrate the cell casing by reacting with sulfhydryl group inside it. Consequently, strains get damaged enough to lose the growth ability of cells (Fig. 10) [25].

Table 3: Bactericidal action of MgO and Cu-doped C₃N₄/MgO.

Samples	<i>S. aureus</i>		<i>E. coli</i>	
	Inhibition Zone (mm)		Inhibition Zone (mm)	
	0.5 mg/50 µl	1.0 mg/50 µl	0.5 mg/50 µl	1.0 mg/50 µl
MgO	1.55	2.05	1.45	1.80
C ₃ N ₄	0	0	0	1.60
2.5% Cu-C ₃ N ₄ /MgO	2.65	4.40	2.60	3.15
5 % Cu-C ₃ N ₄ /MgO	3.45	5.35	3.30	3.40
7.5% Cu-C ₃ N ₄ /MgO	3.95	6.45	3.65	3.85
10% Cu-C ₃ N ₄ /MgO	4.05	7.05	3.95	4.15

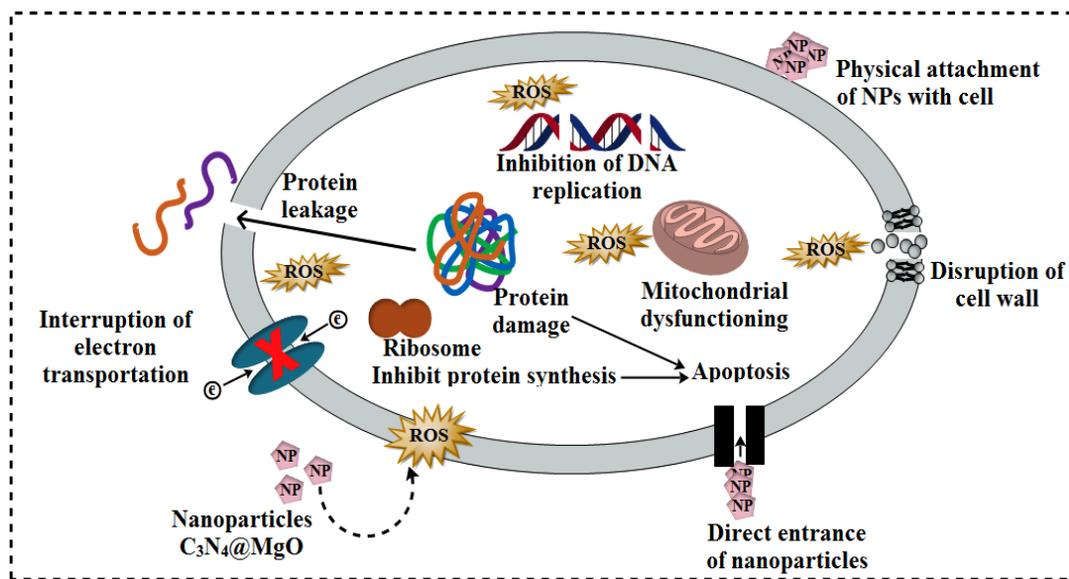


Figure 10: Antimicrobial reaction mechanism of prepared sample.

4. CONCLUSION

Novel Cu-C₃N₄/MgO were prepared through co-precipitation method for dye degradation and antibacterial activities and several properties including structural, morphological and optical were investigated. MgO nanocomposites exhibited FCC cubic structure and transformed itself into nanorods upon Cu and C₃N₄ doping. Doping effects of Cu and C₃N₄ emerged in the form of peak broadening and minor shift to higher angles as shown by XRD results. In FTIR, broad band range of 3040–3550 cm⁻¹ indicated the formation of MgO bond while 620- 873 cm⁻¹ band was ascribed to MgO bond vibration. UV-Vis spectroscopy demonstrated that MgO showed absorption in region 230-310 nm accompanied by redshift resulting in noteworthy decrease in E_g upon doping of Cu and C₃N₄. PL spectra showed emission at 370 nm with a prominent decrease in intensity upon Cu and C₃N₄ doping. XPS confirmed strong signals of C, N, O, and Cu composition with binding energy modifications of Cu-doped C₃N₄-MgO nanorods. DSC analysis

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4 exhibited that the endothermic regions are shifted from 144 °C towards high temperature range
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6 (185°C) upon doping. PCA results revealed that 2.5% Cu-C₃N₄/MgO showed most dye
7
8 degradation in neutral, basic and acidic mediums. Antibacterial performance investigated by disc
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10 diffusion method indicated that maximum dopant 10% Cu-C₃N₄/MgO showed best performance
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12 against *S. aureus* and *E. Coli* at both high and low dose concentrations.
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33 **CONFLICT OF INTEREST STATEMENT**

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36 This manuscript has no conflict of interest.
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