

Revolutionizing material science: Enhanced functionalities through reduced graphene oxide/Al₂O₃/CuO/TiO₂ nanocomposites

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ABSTRACT

Reduced graphene oxide@Al₂O₃-CuO-TiO₂ (ACT) based nanocomposites (NCs) were combined by regulated hydrothermal technique to create novel rGO@metal oxides-based NCs. The resultant NCs showed excellent photocatalytic, antibacterial, anticorrosive, and magnetic characteristics. The use of FTIR, TEM, UV-visible, X-ray diffraction, and SEM aids the structural examination of NCs. The synergistic pairing of ACT NPs with rGO exhibits enhanced photocatalytic, magnetic, anticorrosive, and antibacterial characteristics. The NCs exhibited paramagnetic character ($\chi = 0.140$) and increased induced current with applied magnetic field. The photocatalytic properties of NCs were examined for decomposing methylene blue dye in UV and Sunlight. 94.7 % and 70.5 % dye degradation was observed under UV and Sunlight after 335 and 110 min. of exposure, respectively. The Zone of Inhibition was examined against *S. aureus* (Gram-positive) and *E. coli* (Gram-negative) bacteria and was found comparable with standard antibiotics (Ampicillin) against *S. aureus* bacterial strain. The NCs show 99 % corrosion inhibition efficiency at a low concentration (10 ppm). The potential applications of ACT@rGO NCs in environmental rehabilitation, the medical field, anticorrosive coatings, and impure water purification, contribute toward the development of advanced nanomaterials-based devices.

1. Introduction

Environmental remediation, sustainable healthcare, and clean water are among the most important worldwide issues that attracted the attention of mankind. Innovative material and technology development are essential as society seeks to overcome these challenges. In this quest, NCs have become a key field with versatile solutions that might be used to solve a wide range of environment-related problems. Graphite, a naturally occurring allotrope of Carbon, is known for its high thermal stability and good electrical conductivity. The van der Waals forces linked the layers of graphite with each other. It is used to manufacture different products consisting of solid lubricants to high-performance electrodes [1,2]. Graphene oxide (GO) can be fabricated from Graphite powder and is made of graphene layers having oxygen-functional groups as impurities. GO is used in applications like medicine delivery, water filtration, and sensors, due to its remarkable strength and reactivity [1,3–9]. GO and rGO are useful materials with

tuneable properties which makes them useful for advanced applications. Functional smart materials made of GO and rGO have significant advantages over the traditional counterparts used in electronics, energy storage, and catalysis [9–19]. Due to their extraordinary electrochemical stability and capacity to improve electron transport, rGO-based NCs have become important [20–23]. rGO has been utilized for applications such as transparent conductive thin films, NCs, and supercapacitors. Graphene structure enhances electrical conductivity and thermal stability without compromising its mechanical strength [3, 24–28]. However, these properties are mitigated due to the phenomena of restacking. Restacking in rGO occurs when the weak interactions among the adjacent layers of rGO diminish the Specific Surface Area (SSA), and approachability of active areas present in rGO and decrease the transport of ions, which limits the rGO in different applications [29–31]. To resolve the issue of restacking, researchers have formulated novel methods such as surface functionalization, formation of nanocrystals, and controlled synthesis processes [32–36]. The objective of

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these approaches is to maximize electrochemical performance and increase the exposure of active sites by retaining the dispersed condition of rGO sheets. By mixing rGO with other nanomaterials, like conducting polymers or metal oxides, it is possible to achieve high electrochemical activity and structural stability of NCs [28,37–43]. The performance (electrochemical) of electrodes can be altered and the rate of restacking can be reduced drastically by chemically altering the surface of rGO [44–47]. TiO₂ NPs have gained attention from their first use as a photocatalyst by Fujishima and Honda [48], across different scientific disciplines due to their wide applications and unique characteristics. Researchers have been investigating the synthesis methods, surface modification, and doping of TiO₂ NPs to change their size, shape, and properties for different applications [49–52]. Due to exceptional photocatalytic characteristics, TiO₂ has been investigated for the conversion of solar energy, the creation of self-cleaning surfaces, and the remediation of the environment. TiO₂ NPs find applications in various sectors and technologies and are currently under investigation to uncover new properties and their potential applications [53–57].

Al₂O₃ NPs have been created by researchers using a variety of techniques, including chemical vapour deposition, hydrothermal, sol-gel, and co-precipitation. By employing various aluminum alkoxide hydrolysis and condensation methods, these procedures carefully control the size and shape of the particles [58]. Al₂O₃ NPs are crucial in a variety of applications, such as antimicrobial [59], energy storage [60], ceramics [61], catalysis, capacitors, and insulators because of their excellent electrical insulating properties, thermal stability, and mechanical strength. They are valuable in applications involving corrosion inhibition because of their well-known resistance to corrosion [62,63]. They are extremely beneficial in applications requiring friction and wear because of their remarkable hardness and resistance to deterioration. Al₂O₃ NPs are also employed in industrial processes, such as petrochemical refining, as a catalyst support to change the speeds of reactions. Moreover, these metal oxide NPs find application in electronics, particularly in semiconductor components, insulating layers, and gate dielectrics [60,64–69]. Ag-doped MgO NCs were studied by Panchal et al. for photocatalytic and antibacterial uses [70]. Bi₂O₃ doped with Cu²⁺ ions has been studied by Sharma et al. for improved photocatalytic applications [71]. The optical and photocatalytic characteristics of TiO₂/SnO₂ NCs have been studied by Sharma et al. [72]. Sehrawat et al. studied the radiative and non-radiative emission by nanomaterials for white light-emitting diodes [73,74]. Sharma et al. have investigated Carbon-like materials as adsorbents for CO₂ gas [75]. Kumar et al. have synthesized SiO₂/CMC/Ag hybrids for special medical applications [76].

The Al₂O₃-CuO-TiO₂ paired by rGO NCs for multifunctional applications such as photocatalysis, microbicidal, corrosion resistant, and nanomaterials with magnetic properties are shown for the first time in this paper. For rGO and Al₂O₃-CuO-TiO₂ NCs, a regulated hydrothermal process was employed. The objective of this integration of NPs with rGO was to use the inherent characteristics of each metal oxide NPs to improve the antibacterial, anticorrosive, photocatalytic, and magnetic properties of nanomaterials. Different methods of analysis, such as UV-visible, X-ray diffraction SEM, TEM, and FT-IR, were employed to investigate the structural and functional characteristics of the synergistic NCs. The results confirmed the combination's increased magnetic characteristics, increased antibacterial activity against Gram-positive bacteria, stronger photocatalytic efficiency, and anticorrosive properties, highlighting the remarkable significance of synthesized NCs. There was significant effectiveness on the part of the nanomaterials. The NCs when subjected to ultraviolet light show good photocatalytic activity. The rGO-based NCs demonstrate a significant corrosion inhibition (CIE) of 99 % at just 10 ppm concentration. Results show the importance of customized nanomaterials in solving difficult problems of the scientific community.

2. Materials and methods

Graphite flakes, (Sigma-Aldrich) Min. assay ≥ 99 %, Mol. wt. 12.01, Grade AR, C. No. 7782-42-5. Sulphuric Acid AR, (CDH) Min. assay ≥ 98 %, Mol. wt. 98.08, Grade AR, C. No. 7664-93-9. Sodium Hydroxide Pellets AR, Mol. wt. 40.00, Grade AR, C. No. 1310-73-2. Zinc Oxide (CDH) Min. assay 99.0 %, Mol. wt. 81.38, Grade AR, C. No. 1314-13-2. Titanium Dioxide (CDH) Min. assay 99.9.0 %, Mol. wt. 79.89, Grade AR, C. No. 13463-67-7. Oxalic Acid (CDH) Min. assay 99.5 %, Mol. wt. 126.07, C. No. 6153-56-6. Aluminum Chloride (CDH) Min. assay 99.9 %, Mol. wt. 133.34, C. No. 7446-70-0. Hydrochloric acid (CDH) Min. assay 37.0 %, Mol. wt. 36.46, grade AR, C. No. 7647-01-0. Nitric acid (Sigma-Aldrich) Min. assay 70.0 %, Mol. wt. 63.01, grade AR, C. No. 7697-37-2 Ethanol (CSS) Ethyl alcohol 99.9 %, AR, CSS reagent.

2.1. Production of rGO

Hummer's method (improved) was followed to fabricate rGO [16]. Graphite powder and KMnO₄ were reacted with sulfuric acid and ortho-phosphoric acid, the reaction was monitored and performed at 85 °C. Hydrogen peroxide and distilled water were then added. After 24 h, the products were separated using centrifugation, followed by ultrasonic cleaning with hydrogen chloride, and then with double distilled water followed by ethyl alcohol.

2.2. Synthesis of Al₂O₃ NPs

Al₂O₃ NPs were prepared by the previously known Co-precipitation method [77]. Aluminum trichloride (AlCl₃) precursor was used to prepare Al₂O₃ NPs. A translucent solution of AlCl₃ was made in 200 ml of distilled water. Afterward, NH₃ was gradually added to the stirred AlCl₃.6H₂O solution until a pH of 9.0 was maintained. Formation of a white ppt. takes place, which was the gelation of Al cations as hydroxides Al(OH)₃. The resultant ppt. was washed using double distilled water and NPs were obtained by the centrifugation method. After being separated, these moist particles were put in an electric oven at 150 °C to remove the moisture content. The compact solid was grounded into a fine powder. The synthesized NPs were heated at 600, 800, and 1000 °C using a muffle furnace. A fine white alumina nanopowder was finally obtained and stored.

2.3. Synthesis of CuO NPs

To produce Copper oxide NPs using the chemical precipitation method, we adhered to a standard procedure [78]. In the process of synthesizing CuO NPs, an initial step involved dissolving CuCl₂.2H₂O (9.0 g) and NaOH pellets (5.4 g) separately in ethyl alcohol. The quantity of ethyl alcohol utilized was minimized to the necessary amount for dissolving Copper (II) chloride dihydrate and sodium hydroxide, individually. Slowly and continually mixing at room temperature, the NaOH solution was added dropwise to the Copper (II) chloride dihydrate solution. A black precipitate was formed as the solution's color varied from green to bluish-green to black, identified as Cu(OH)₂. The ppt. was subjected to filtration using a centrifuge (Centrifuge Make 5702R, Germany) and subsequently cleaned with deionized water and ethyl alcohol to eliminate the chloride from the resulting ppt. The resulting ppt. was dried in an oven at 50 °C. After that solid ppt. were heated at 200 °C, 400 °C, and 600 °C to obtain crystalline CuO-NPs. The heat-treated product was crushed to obtain solid black powder NPs.

2.4. Synthesis of TiO₂ NPs

The sol-gel method is used in the processing of synthesized TiO₂ NPs. Samples were labeled as solutions A and B, which must be created in accordance with the procedure and combined at a temperature that has been specified. The initial solution, Solution A, was employed by

selecting 0.5 mol of TiO_2 in 100 ml of double-distilled H_2O . The solution was made more acidic using HNO_3 . 100 ml of a solution containing 0.1 M di-hydrated oxalic acid and ethyl alcohol (solution B). Throughout the entire process, the temperature was fixed at 70°C . In the first six hours, a gelatinous mixture was produced. The product was dried for twenty-four hours at 100°C . Following a 6 h drying period, the products were cleaned with acetone and water.

2.5. Production of rGO@ACT NCs

An *ex-situ* method was used to dope the rGO with NPs of Al_2O_3 , CuO, and TiO_2 . The hydrothermal technique was performed at high pressure and temperature. Al_2O_3 (0.25 M), CuO (0.25 M), TiO_2 (0.25 M), 0.5 M NaOH, and 0.5 g of rGO were used for the fabrication of NCs.

The NaOH solution was combined with prepared rGO and the respective NPs (TiO_2 , Al_2O_3 , and CuO). The mixture was ultrasonically treated for 15 min for the best possible dispersion and homogeneity. A hydrothermal bomb was carefully filled with the resulting mixture. Thermal treatment for the hydrothermal device involved 24 h at 150°C in an oven. Centrifugation was used to extract the NCs material from the reaction mixture, and contaminants were completely removed by washing with double distilled water. The NCs material was dried at 50°C and stored.

2.6. Cell susceptibility assay

Spot Assay: To assess the antimicrobial potential of synthesized compound. We performed the cell susceptibility assay on *E. coli* bacterial strain and *S. aureus* (MSSA 29213). A fixed amount of synthesized compound (3 mg) was used for the antimicrobial potential of tested compounds by spot assay. For this, *S. aureus* and *E. coli* cells were grown till the mid-log stage in Luria Bertani (LB) and Mueller Hinton agar (MHA) broth, respectively after 2-3 folds revivals. An approx. 0.001 million cells were plated on MHA and LB-agar plates. Different amounts of tested compounds were spotted on plates to assess their antimicrobial potential against tested microbial strains. With a positive control, Ampicillin (20 μg) was used. After overnight incubation at 37°C , the zone of inhibition (ZOI) was observed.

2.7. ACT@rGO NCs: Photocatalytic study

To investigate NCs' photocatalytic activity on organic dyes, the UV-visible spectrophotometric method was employed. (UV-2600, Mumbai; Shimadzu; Toshvin Analytical). The dye was exposed to a concentration of 100 ppm NCs, and the absorbance was measured at different intervals. UV lamps (A and B) were utilized to expose the dye and solution containing NCs. The photocatalytic activity was performed in the presence of sunlight, and halogen lamps producing UV A and B radiations, (75 W and 100 Luman intensities) make BURAQ. For photocatalytic research, a 100 ppm concentration of NCs was obtained with 30 mg/L of MB dye. The sample within the chamber is kept 20 cm away from the halogen bulb. Ice bath is also utilized to avoid evaporation and thermal degradation of dye.

2.8. ACT@rGO NCs: Magnetic study

The magnetic investigation employed Gouys balance to ascertain the magnetic susceptibility and paramagnetic character of the NCs. A weight shift was seen after exposing the NCs to different magnetic field strengths. SES Instruments (GMX-02), Haridwar, India was used for magnetic characterization. A basic matrix called magnetic susceptibility is used to measure a material's innate ability to become magnetized in response to an applied magnetic field. The methodology used in the experiment includes a variety of sample arrangements, such as a glass tube filled with powder or a long empty tube submerged in a solution of the sample. The sample is positioned such that one portion is always

exposed to a constant magnetic field and the other part is in a weak or nonexistent magnetic field. Notable findings are obtained by quantifying the ensuing forces using a balance to increase precision. The sample's mass is ascertained both in the presence and absence of a magnetic field. The magnetic susceptibility is then ascertained by analyzing the weight variations.

The experimental method has several stages that must be carried out in sequence. The NCs material is subsequently placed inside the tube. Next, a magnetic field is generated, and an accurate weight measurement is carried out. To check the reproducibility, experiments were performed seven times. The generated electric current's magnitude was adjusted each time to obtain several data points. The weight and magnetic field variations are recorded in the measurements for every reading taken. The resulting difference in weight between the two objects is then converted from grams to milligrams. Moreover, the computation of the difference between successive magnetic fields follows a similar procedure to that utilized for weight differences, except that the differences are squared to make further analysis easier. To facilitate the computation of the slope, a graph is subsequently created to show the link between the weight change and the H^2 .

2.9. ACT@rGO NCs: Anticorrosive study

To find the anticorrosive nature of ACT@rGO NCs in 1.0 N H_2SO_4 medium at STP, research was conducted on mild steel (MS) samples. After adding ACT@rGO NCs, MS (97.0 % Fe) of a fixed size and weight was precisely weighed and subjected to a corroding medium. A stock solution of NCs (100 ppm) was prepared in the corroding medium and further concentrations of NCs were prepared from stock solution by dilution method. The weight of coupons after corrosion experiments was accurately recorded after a 13 h exposure to a corrosive liquid. The Corrosion Inhibition Efficiency (CIE) was calculated using standard ASTM procedure.

3. Results and discussion

3.1. Absorption study of ACT@rGO NCs

The metal oxide NPs have been examined utilizing UV spectroscopy because their size is crucial to their intended applications. Interpreting the electrical properties of the NCs, an optical band gap was observed using UV-Vis spectra. UV transitions in the molecules present in the sample show an absorption peak. ACT@rGO NCs' UV-visible spectra are shown in Fig. 1. Tauc charts illustrating the ACT@rGO NCs' direct band gap are shown in Fig. 2. UV-visible spectroscopy reveals metal oxide

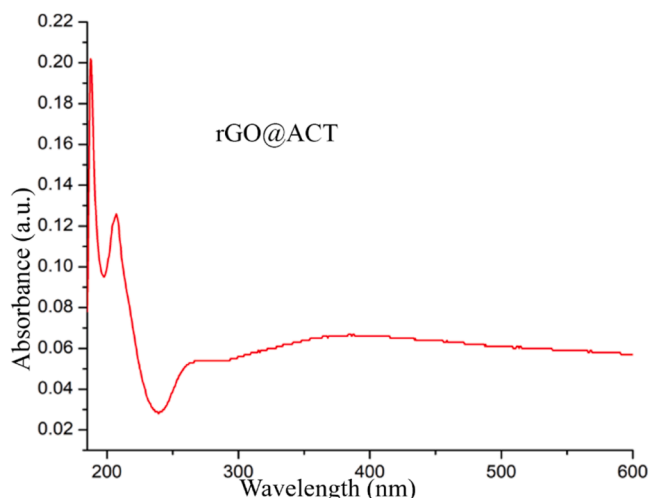


Fig. 1. Absorption spectra for ACT@rGO NCs.

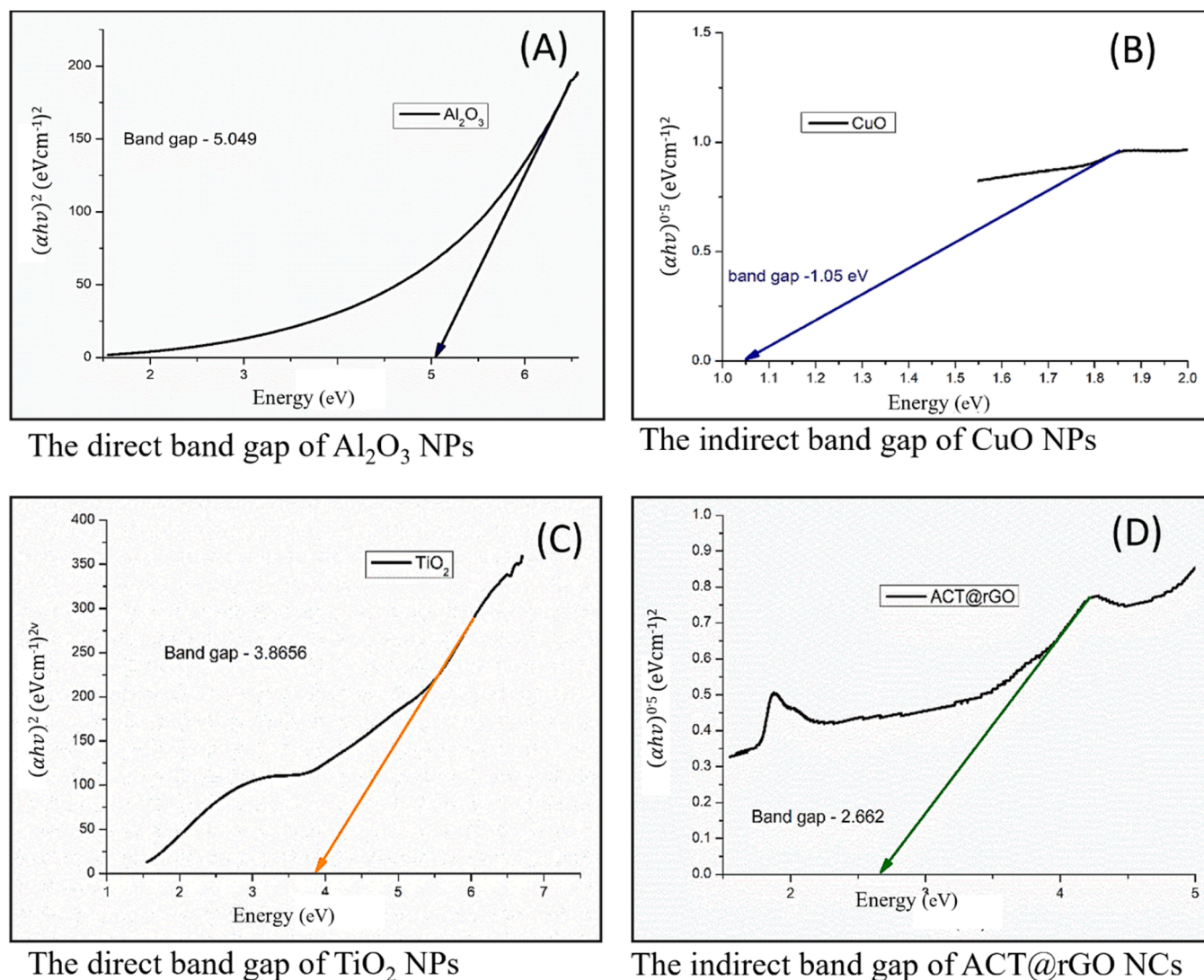


Fig. 2. Band gap (Direct and indirect) of Al_2O_3 (A), CuO (B), TiO_2 NPs (C), and ACT@rGO NCs (D), respectively.

adsorption less than 200 nm. There is a change in NCs absorption when metal NPs are added to the rGO matrix.

The direct and indirect band gap of both NPs and ACT@rGO NCs was calculated by analyzing their absorption spectra using a Tauc equation. The Tauc equation was used for finding optical band gaps in semiconductor materials. The Tauc equation gives the relation of $h\nu$ to the absorption coefficient, α in a semiconducting material.

The Eq. (2) was used to find the band gap:

$$\alpha h\nu = A(h\nu - E_g)^n \quad (2)$$

The band gap value is attained by extrapolating the linear section of the Tauc curve.

Depending on the n value, the band gap (direct and indirect) energy (E_g) is represented by the X-axis intercept.

The band gap of Al_2O_3 , CuO , TiO_2 NPs, and ACT@rGO NCs are depicted in Fig. 2, respectively.

The observed band gap of the NCs (2.662 eV) was found smaller than all individual metal oxide NPs ($\text{Al}_2\text{O}_3 = 5.03$ eV, and $\text{TiO}_2 = 3.865$ eV) which can be due to several reasons. The first probable reason is due to the formation of the heterojunction. When two or more semiconductors with different optical band gaps come in contact, they create heterojunctions. These interfaces can lead to the alignment of band edges, resulting in a reduction of the overall band gap. The lower optical band

gaps of CuO (1.05 eV) and TiO_2 (3.86 eV) likely influence the final band gap of the NCs. The second probable reason is the formation of e^-/h^+ transfer. The migration of e^- and holes generated from light occurs due to a small optical band gap. For example, electrons excited in CuO with its lower optical band gap migrate to the CB of TiO_2 , reducing the recombination rate and enhancing photocatalytic activity. The third probable reason is doping. The foreign elements or defects within the NCs can form fresh energy levels in the bandgap, further narrowing the band gap. Such defects act as trapping centers for excited e^- and holes, further promoting their separation and utilization in photocatalytic reactions.

3.2. FTIR spectroscopic investigation of ACT@rGO NCs

Individual FT-IR characterization of NPs and rGO NCs was done. Fig. 3 depicts FTIR of CuO (Fig. 3 A), Al_2O_3 (Fig. 3 B), and TiO_2 NPs (Fig. 3 C). The FTIR peaks observed for CuO NPs are interpreted. The FTIR peaks at 525 and 588 cm^{-1} were attributed to Cu-O stretching vibrations in the CuO lattice. FTIR peaks suggest the presence of Cu in the +2-oxidation state, confirming CuO formation. The splitting of the FTIR peak around 588 cm^{-1} is often observed and could be related to different oxygen environments around the Copper ions.

The minor FTIR peak of 3389 cm^{-1} (broad and small) corresponds to O-H stretching vibrations of adsorbed water molecules. CuO NPs have a

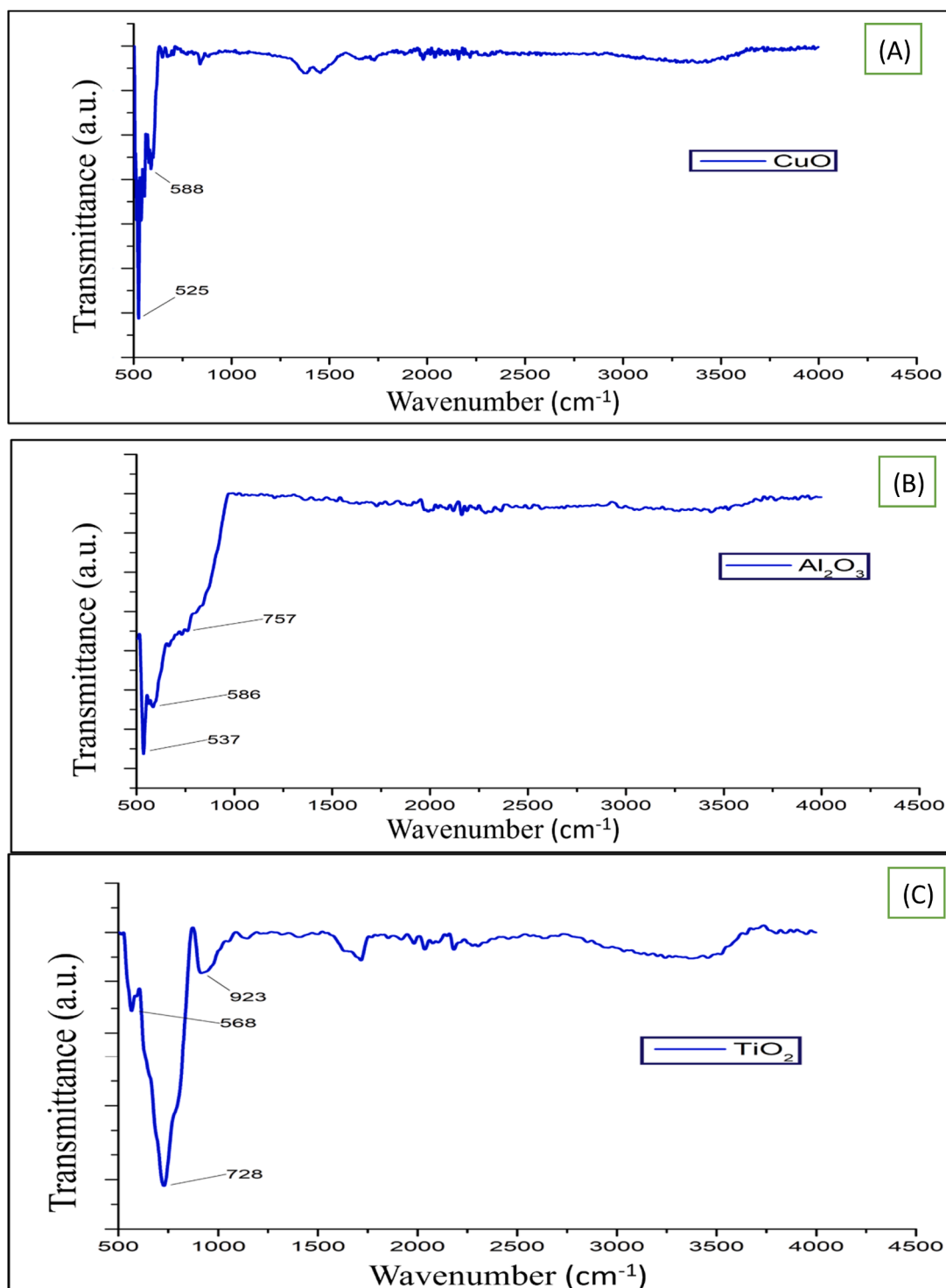


Fig. 3. FTIR spectra of CuO (A), Al_2O_3 (B), and TiO_2 NPs (C).

significant surface area, making them prone to water adsorption.

The presence of strong Cu-O stretching FTIR peaks supports the successful synthesis of CuO NPs.

The broad O-H peak indicates surface water adsorption, which is common in NPs.

The absence of significant FTIR peaks in other regions suggests the purity of CuO NPs, supported by further characterization by XRD.

Al-O FTIR signal appears at 787 cm^{-1} . The existence of the most stable polymorph at high temperatures, that is, the $\gamma\text{-Al}_2\text{O}_3$ phase, is possible. $\gamma\text{-Al}_2\text{O}_3$ may also be indicated by the Al-O-Al peak appearing in

the FTIR spectra at 586 cm^{-1} . It could have to do with flaws or the hydroxyl groups on the NPs' surface. Concerning the FTIR peaks that have been identified, the strong peak at 787 cm^{-1} and possible Al-O-Al at 586 cm^{-1} suggest that the main phase in Al_2O_3 NPs is most likely $\gamma\text{-Al}_2\text{O}_3$. Elevated annealing temperatures promote the production of $\gamma\text{-Al}_2\text{O}_3$. The $\gamma\text{-Al}_2\text{O}_3$ interpretation is strengthened if identical FTIR peaks are seen at 600 $^\circ\text{C}$, 800 $^\circ\text{C}$, and 1000 $^\circ\text{C}$.

The FTIR spectra of TiO_2 NPs were also taken. A prominent FTIR peak at 569 cm^{-1} is characteristic of Ti-O stretching vibrations in the Anatase phase of TiO_2 . It's a strong indicator that TiO_2 NPs primarily

consist of the Anatase form, which is the most common photocatalyst form of TiO_2 . An FTIR peak at 729 cm^{-1} is typically associated with O-Ti-O bending vibrations in the Anatase structure, further supporting the presence of the Anatase phase. A peak at 924 cm^{-1} occurs due to Ti-O stretching vibrations in a minor Rutile phase, which can sometimes coexist with the Anatase phase, especially at higher annealing temperatures. A small and broad FTIR due to O-H stretching from adsorbed H_2O on the NPs surface was observed at 3362 cm^{-1} .

The FTIR spectrum of hydrothermally synthesized NCs containing Al_2O_3 , CuO, TiO_2 , and rGO reveals interesting details about its functional groups and chemical bonding. Fig. 4 depicts FTIR spectra for ACT@rGO, carboxylate-metal bonds, or methyl group bending, indicating that the NCs contain rGO. O-H stretching vibrations are present in the wide and strong FTIR signal at 3441 cm^{-1} , which is caused by surface hydroxyl groups on adsorbed water molecules, TiO_2 , and Al_2O_3 . The C=C stretching vibrations of the aromatic rings in rGO are responsible for an FTIR signal at 1635 cm^{-1} , indicating that the molecule was successfully incorporated into the NCs.

The C=O stretching vibrations of carboxylic acid groups or carbonyl moieties on the surface of rGO may be the cause of the FTIR signal at 1733 cm^{-1} . The FTIR spectrum's peak at 1393 cm^{-1} , which is most likely caused by amides.

More relevant possibilities for rGO showing a peak at 1393 cm^{-1} may be due to defective Graphene synthesized. While rGO generally aims to restore the sp^2 character of graphene by removing oxygen-containing functional groups in GO, it's not always a perfect process. Some residual oxygen functionalities or defects can remain in the rGO structure. A peak around 1393 cm^{-1} in the rGO spectrum can potentially be attributed to these remaining C-H deformations on the aromatic ring or residual carboxyl groups (COOH) on the defect sites.

The FTIR peaks at 580 cm^{-1} and 707 cm^{-1} indicate a possible association with Al-O and Ti-O vibrations in the corresponding metal oxides, suggesting the successful incorporation of these oxides into the NCs.

The presence of small FTIR peaks at 1002 , 1099 , and 1232 cm^{-1} could be due to distinct C-O stretching originating from alkoxy or epoxy groups on rGO. The presence of additional FTIR peaks in peak positions compared to individual components indicates the potential for interactions between the phases in the NCs.

Overall, the FTIR spectrum confirms the presence of all constituent phases in the rGO-based NCs and suggests potential interactions between metal NPs and NCs. The observed functional groups provide valuable insights into the surface chemistry and possible bonding mechanisms within the composite.

3.3. XRD study of ACT@rGO NCs

The structural feature, size, shape, crystallinity, crystal parameters, and morphology of NCs was studied by X-ray diffraction technique. The P-XRD of rGO-based NCs is shown in Fig. 5. The XRD peaks (10.08 , 25.36 , 26.72 , 35.62 , 37.86 , 38.72 , 42.5 , 48.06 , 53.9 , 55.08 , 62.72 , 70.32 , and 75.06°) offer valuable insights into the crystal structure and phase composition of hydrothermally synthesized NCs containing Al_2O_3 , CuO, TiO_2 , and rGO. Peaks at 25.36° , 35.62° , 37.86° , 38.72° , 53.9° , and 70.32° can be attributed to the JCPDS card No. 46-1315 for γ -alumina (γ - Al_2O_3), indicating its presence in the NCs [58–62]. The peaks at 42.5° , 55.08° , and 62.72° correspond well with the JCPDS card No. 80-1917 for Tenorite CuO, suggesting its successful incorporation into the NCs [71–73]. Peaks at 26.72° , 48.06° , and 75.06° align with the JCPDS card No. 21-1272 for anatase TiO_2 , implying its inclusion in the NCs structure [49–52]. The absence of a distinct peak for rGO is expected due to its amorphous nature. However, the broad hump around 10° could be attributed to the (002) plane of rGO, indicating its successful exfoliation and incorporation into the composite matrix.

The observed peak shifts compared to the standard JCPDS patterns hint at potential interactions between the component phases. Overall, the XRD data confirms the successful synthesis of the rGO-based NCs containing Al_2O_3 , CuO, TiO_2 , in the rGO matrix in their respective crystalline phases. The observed peak shifts suggest potential interactions between the components, NPs, and rGO NCs.

3.4. FESEM study of ACT@rGO NCs

The morphology, particle size, distribution, agglomeration, surface roughness, interfacial bonding, and other characteristics of the NPs in the rGO sheet were all determined using the FESEM approach. FESEM pictures of ACT@rGO NCs at various magnifications are displayed in Fig. 6.

Fig. 7 depicts selected area diffraction and EDX elemental analysis of ACT@rGO NCs. The NCs show amorphous character due to the presence of the rGO matrix. A sheet-like spongy structure is visible in SEM images of NCs. Alumina, CuO, and TiO_2 NPs were perfectly entrapped in the rGO matrix as seen from SEM images at X 30,000 and X 75,000 magnification. The average particle size ranges from 100 to 120 nm. There is a uniform distribution of particle size and morphology of NCs. The highly porous nature and large surface area make these NCs suitable for adsorption, catalytic, and molecular sieve characteristics.

Selected area diffraction and EDX elemental analysis of ACT@rGO

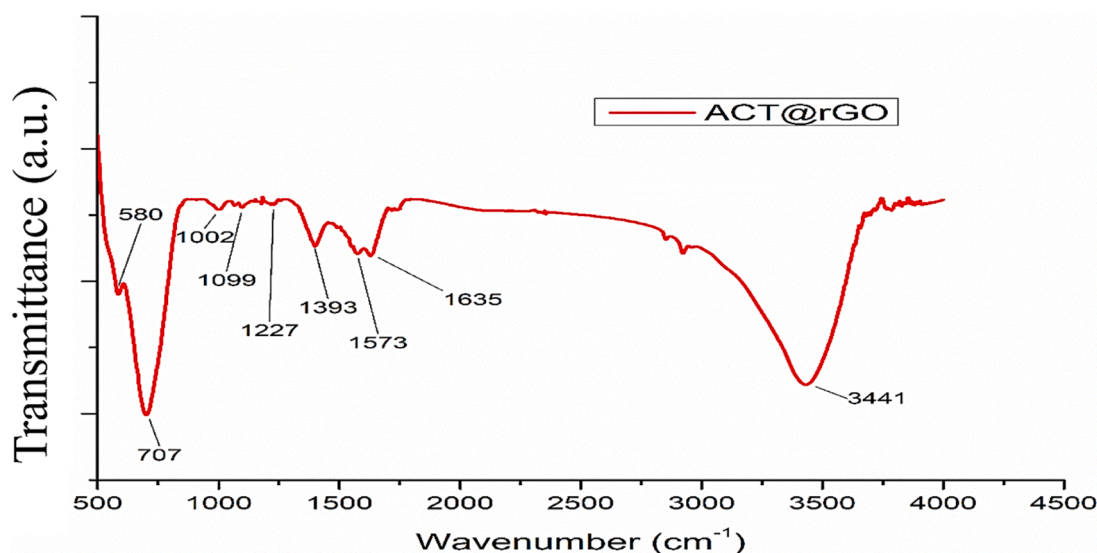


Fig. 4. FTIR Spectra for ACT@rGO NCs.

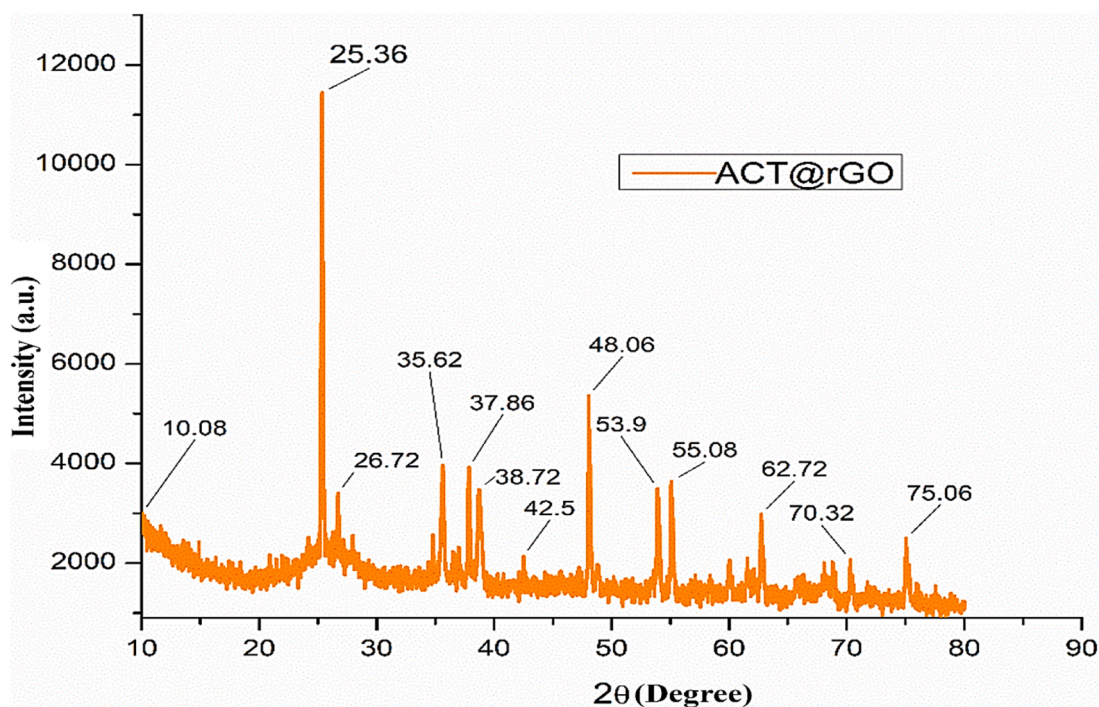


Fig. 5. PXRD of ACT@rGO NCs.

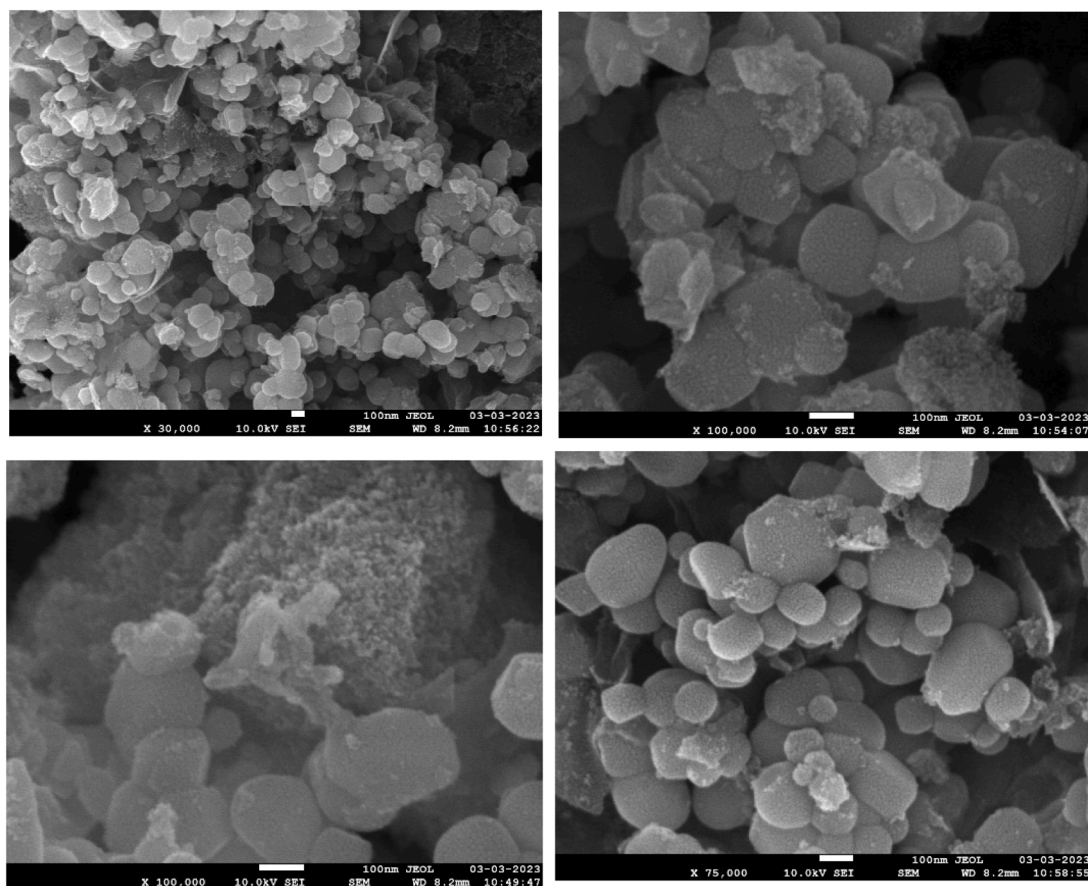


Fig. 6. FE-SEM of ACT@rGO NCs.

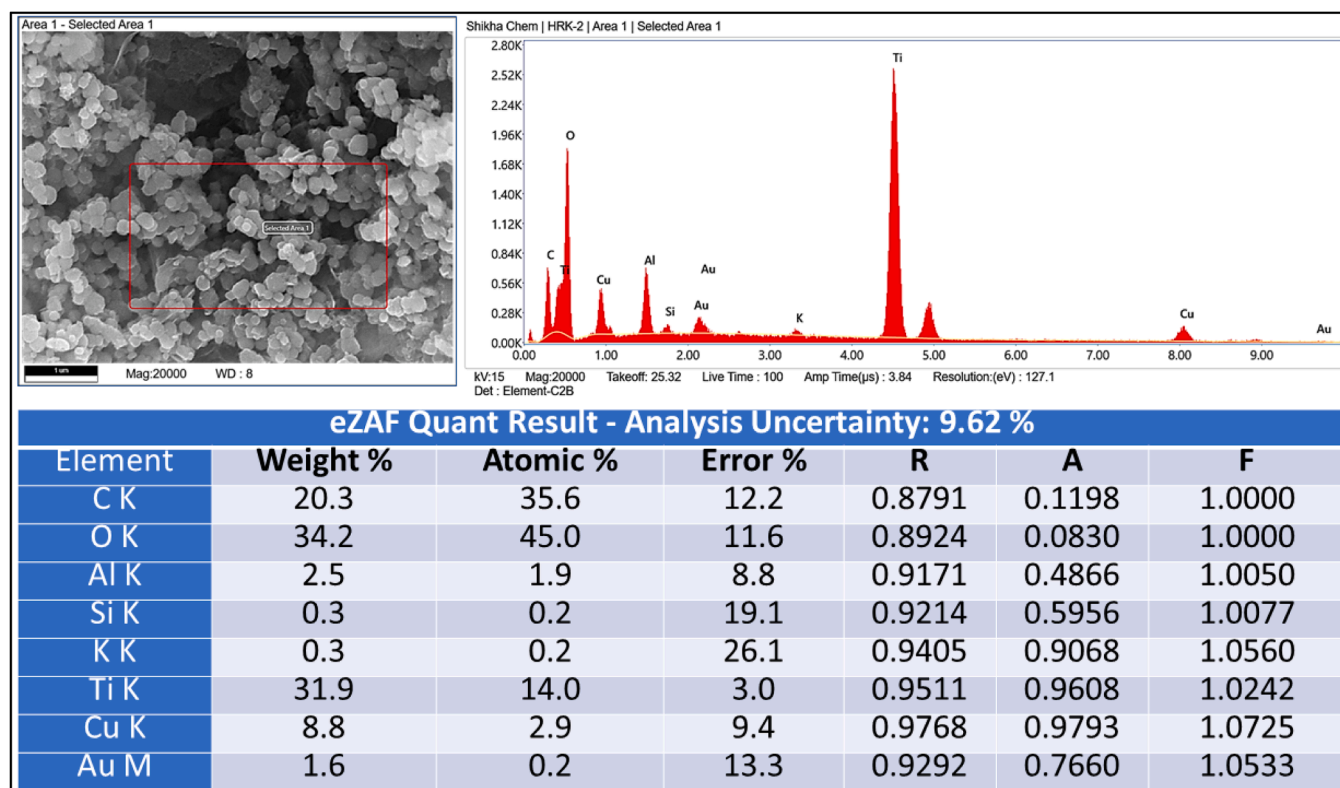


Fig. 7. Selected area diffraction and EDX elemental analysis of ACT@rGO NCs.

NCs (Fig. 7) depicts the major wt. percentage of Carbon, Oxygen, and Titanium elements. Aluminum (2.5 %) and Copper (8.8 %) were present in lesser amounts. Few trace elements (K and Si = 0.3 %) were also seen in EDX elemental analysis present as impurities.

3.5. TEM images for ACT@rGO NCs

TEM study of NCs was carried out to examine the morphology of individual NPs and NCs altogether. The rGO-based NCs look like flat sheet-like structures in which metal NPs are completely embedded in the rGO network. Fig. 8 depicts TEM images of ACT@rGO NCs. The average particle size of NCs matched with the size obtained from FESEM images and was 100 to 120 nm. NPs are uniformly distributed in the rGO sheet. No aggregation or accumulation of NPs was observed in NCs. The Alumina, TiO₂, and CuO NPs can be clearly distinguished depending on different brighter and dark shades due to variations in electron density around metal atoms. The electron diffraction pattern reveals the crystalline structure of individual NPs but NCs as a whole are amorphous. Defects or any structural irregularity were not observed in TEM images of rGO-based NCs. Overall synthesized NCs were homogeneous and porous, NPs were uniformly distributed in the rGO network depicted by a regular distribution of black and white color in the matrix. No specific functional groups can be seen on the surface of NCs as indicated by no changes in contrast at the surface and bulk of NCs. It is seen from TEM images that an appropriate synthesis method, purification, filtration, and drying process was adopted in synthesizing the NCs as depicted from defects-free NCs. The broadening of concentric rings in the SAED pattern represents the polycrystalline nature of NPs.

4. Applications of ACT@rGO-based NCs

4.1. ACT@rGO NCs: Antibacterial study

Antibacterial activity of ACT@rGO NCs was investigated against

both Gram-positive (*S. aureus*) and Gram-negative (*E. coli*) bacteria. Results from the spot assay revealed that compound ACT@rGO exhibited potent antibacterial activity against *S. aureus* (MSSA 29213). The assay, conducted with increasing concentrations of ACT@rGO ranging from 0.5 mg to 3 mg, demonstrated a concentration-dependent effect, with a distinct and measurable Zone of inhibition observed in a concentration-dependent manner (Fig. 9). In Fig. 9, the ACT@rGO NCs show the antimicrobial activity against *S. aureus* bacterial strain. Importantly, ACT@rGO did not show any significant antibacterial effect against *E. coli*, indicating a specificity of action against Gram-positive bacteria. The zone of inhibition shown by ACT@rGO NCs was comparable to standard antibiotic ampicillin at 3 mg/mL. The maximum concentration of ampicillin was 5 µg/µL which is equivalent to 3 mg/mL of NCs in terms of ZOI. The structural differences between Gram-positive (e.g., *S. aureus*) and Gram-negative (e.g., *E. coli*) bacteria influence the antibacterial activity of the NCs. Gram-positive bacteria have a thick peptidoglycan layer in their cell walls, which might interact differently with the NCs compared to Gram-negative bacteria, which have an outer membrane that could affect permeability and sensitivity to the NCs. The presence of metal oxides (Al₂O₃, CuO, TiO₂) in the NCs might generate reactive oxygen species (ROS) more effectively against one type of bacteria over the other, due to differences in cell wall composition and thickness. A higher Zone of inhibition obtained in the case of *S. aureus* further supports structural differences between the two bacteria. These results underscore the promising antibacterial potential of the ACT@rGO NCs, suggesting its consideration for further exploration and development as a targeted agent against *S. aureus* infections.

4.2. Magnetic properties of ACT@rGO NCs

The weight change (ΔW) of ACT rGO concerning H^2 is displayed in Fig. 10. The weight of the vacant tube (a) was 12.263 g. The magnetic susceptibility (χ) was calculated using the Eq. (3).

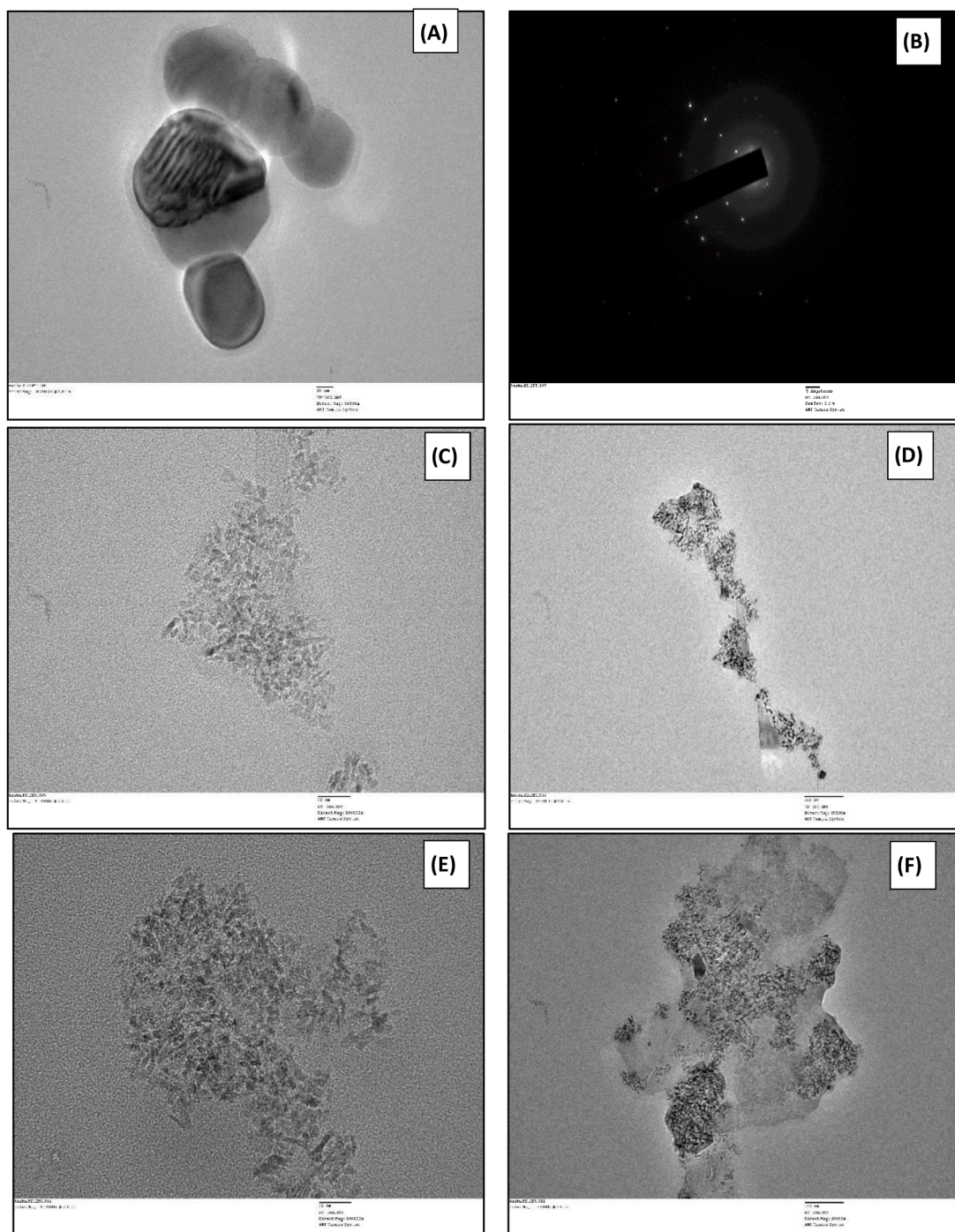


Fig. 8. TEM of ACT@rGO NCs (A-F). Five enlarged rGO NCs (A), SAED pattern of NCs (B), TEM of ACT@rGO NCs at diverse magnification and angles (C-F).

$$\chi = \frac{2g}{A} \times \frac{\Delta W}{H^2} \quad (3)$$

Here, W = Wt. of NCs filled in a glass tube.

ΔW = Wt. difference of NCs.

$$\chi = \frac{2 \times 980 \times 0.0013}{0.2 \times 90695} \quad (4)$$

Eq. (3) yielded χ of 0.14005, falling within the range of NCs' paramagnetic characteristics [43]. The produced ACT@rGO NCs were hence paramagnetic.

4.3. ACT@rGO NCs: Photocatalytic study

The current study used UV-visible spectroscopy performed at regular intervals to investigate the photocatalytic degradation of MB dye by the NCs. The fluctuation of absorbance for ACT@rGO NCs for breaking down methylene blue (MB) dye under UV radiation is shown in Fig. 11 along with the exposure period. The results show a statistically significant decrease in absorbance as well as in the MB solution after the sample was exposed to UV-A and UV-B radiation from a 75 W halogen lamp. The original blue color of the solution changed to a paler tint, indicating dye degradation.

Remarkably, the decrease in absorbance at the maximum wavelength of MB dye (ϵ -max = 668 nm) in our study demonstrated a steady

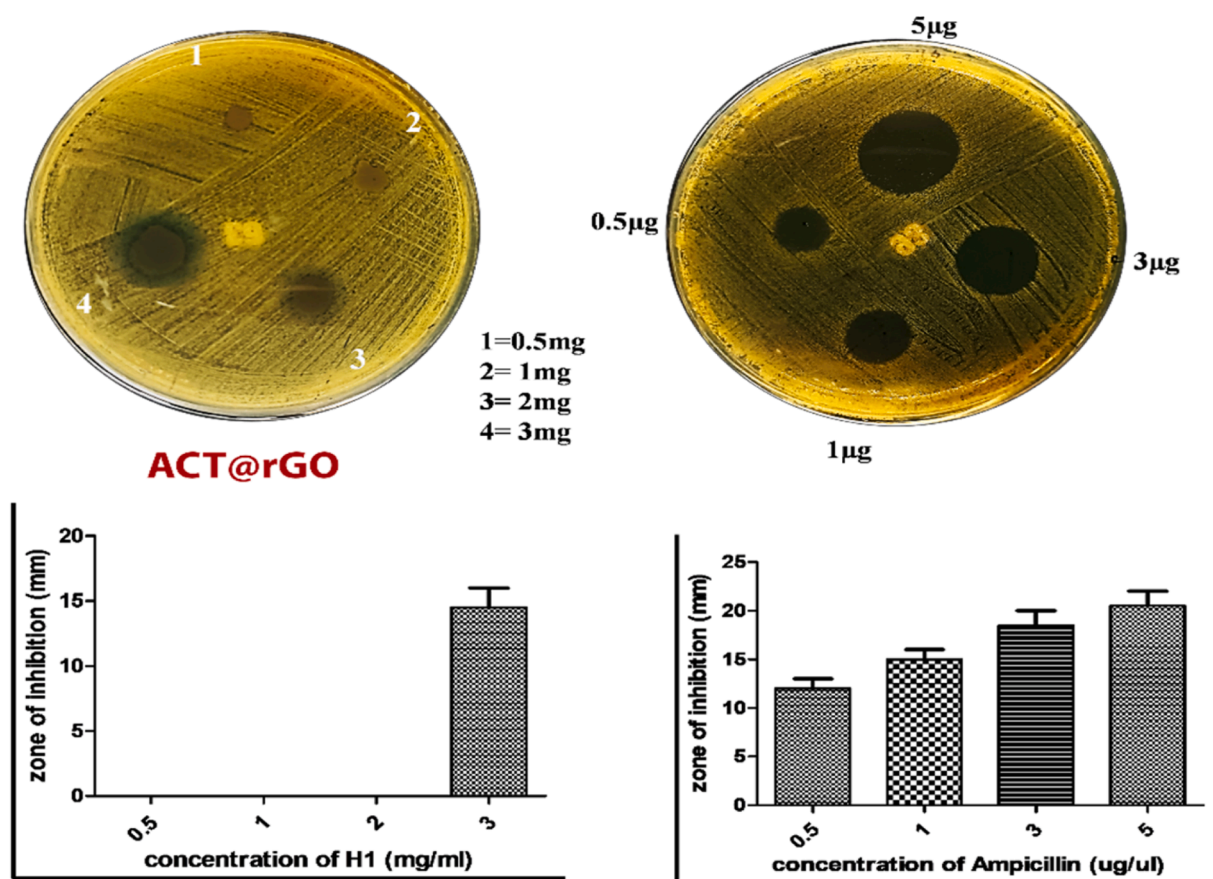


Fig. 9. Potent antimicrobial activity of ACT@rGO NCs investigated on *S. aureus*.

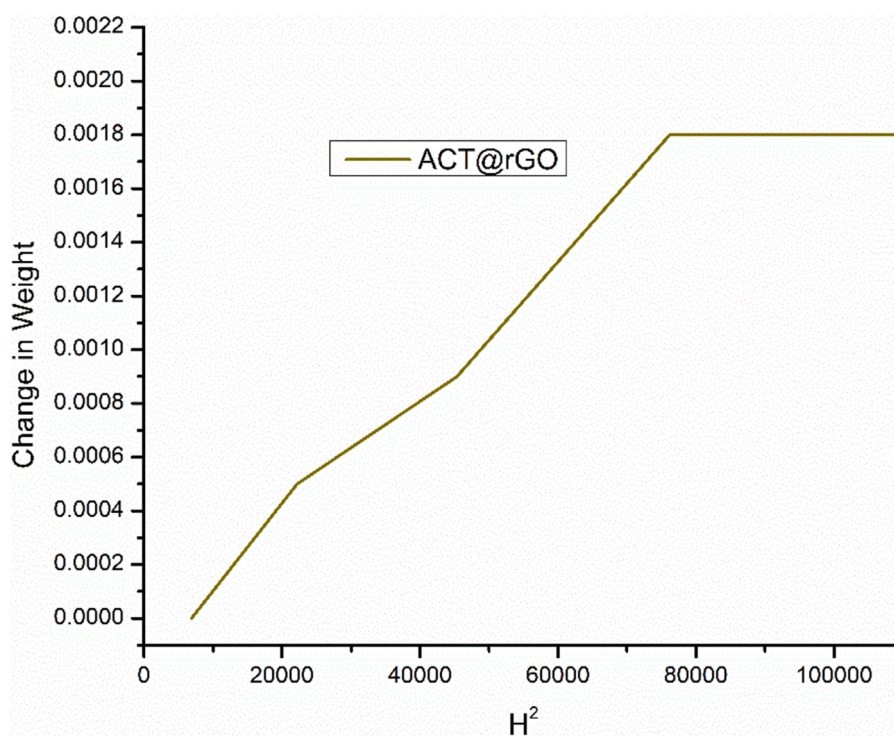


Fig. 10. Weight change versus the applied magnetic field investigated against ACT@rGO NCs.

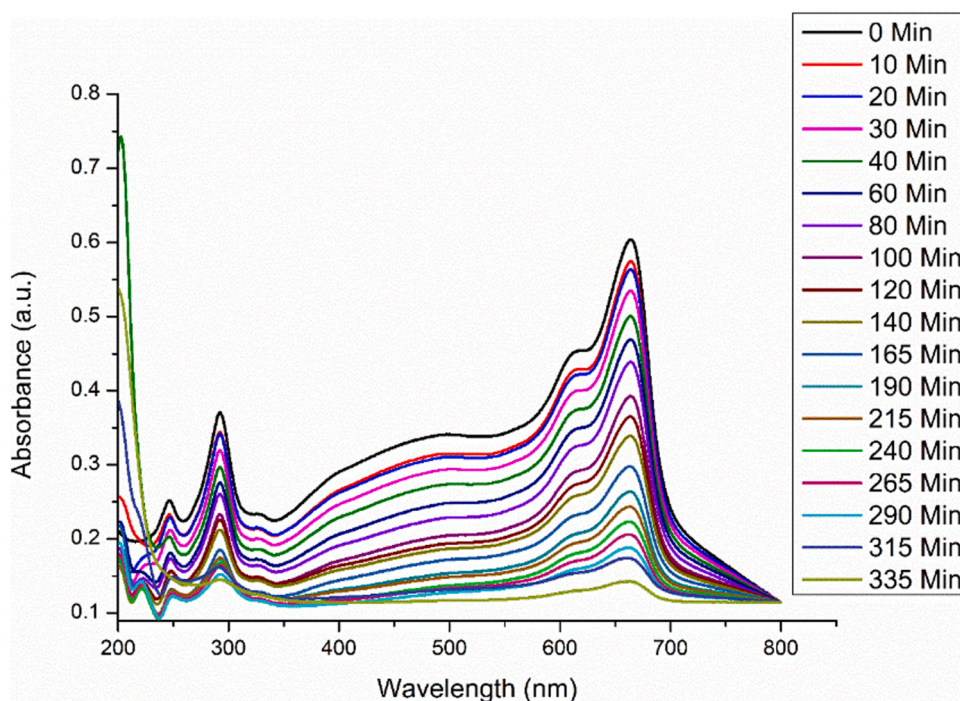


Fig. 11. Variation of absorbance with exposure time for ACT@rGO NCs for degrading methylene blue dye under UV radiation.

drop in the dye's concentration. Furthermore, the solution's pH showed a corresponding decline, indicating the formation of acidic byproducts during the photocatalytic degradation [79]. The study's findings demonstrate how long the wavelength of UV light breaks down MB dye, suggesting a potential use for this dye in wastewater treatment and environmental remediation processes [80]. MB dye was degraded by 94.72 % in 335 min. under irradiation from a halogen lamp of 75 W emitting UV-A + UV- B radiations. In the context of pollution removal, the present work makes advancement to the understanding and use of photocatalytic techniques. It creates a strong foundation for further studies in this field.

In visible light, ACT@rGO NCs were also the subject of a photocatalytic investigation. After 110 min, MB dye had degraded by 70.5 %. A concentration of 100 ppm of NCs was employed together with 30 mg/L of MB dye. Fig. 12 shows how the absorbance of ACT@rGO NCs

changes over time when they are exposed to white light to break down MB dye.

Mechanism of dye degradation

Fig. 13 depicts the breakdown pathway of MB dye. The following mechanism describes the different stages that the $\text{Al}_2\text{O}_3\text{-CuO-TiO}_2\text{-rGO}$ NCs go through to decompose MB dye:

Creation of e^- -hole Pairs:

Photons with energy higher than the NCs' bandgap are absorbed by the $\text{Al}_2\text{O}_3\text{-CuO-TiO}_2\text{-rGO}$ when exposed to light, which results in the creation of e^- -hole pairs [42]. $h\nu$ (light) + $\text{Al}_2\text{O}_3\text{-CuO-TiO}_2\text{-rGO} \rightarrow e^-$ (electron) + h^+ (hole) h^+ + Methylene Blue dye $\rightarrow$ Dye degraded products.

An electron's reduction: The produced electrons (e^-) take part in reduction processes concurrently. They could react with the system's oxygen or other species [41]:

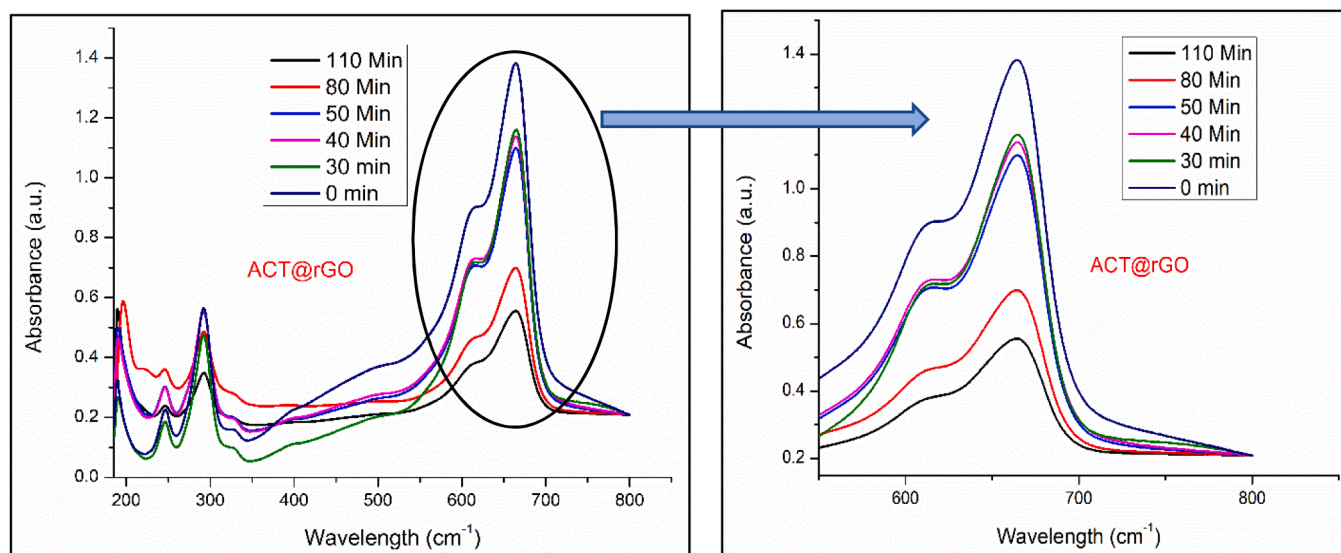


Fig. 12. Variation of absorbance with exposure time for ACT@rGO NCs for decomposing MB dye in Sunlight.

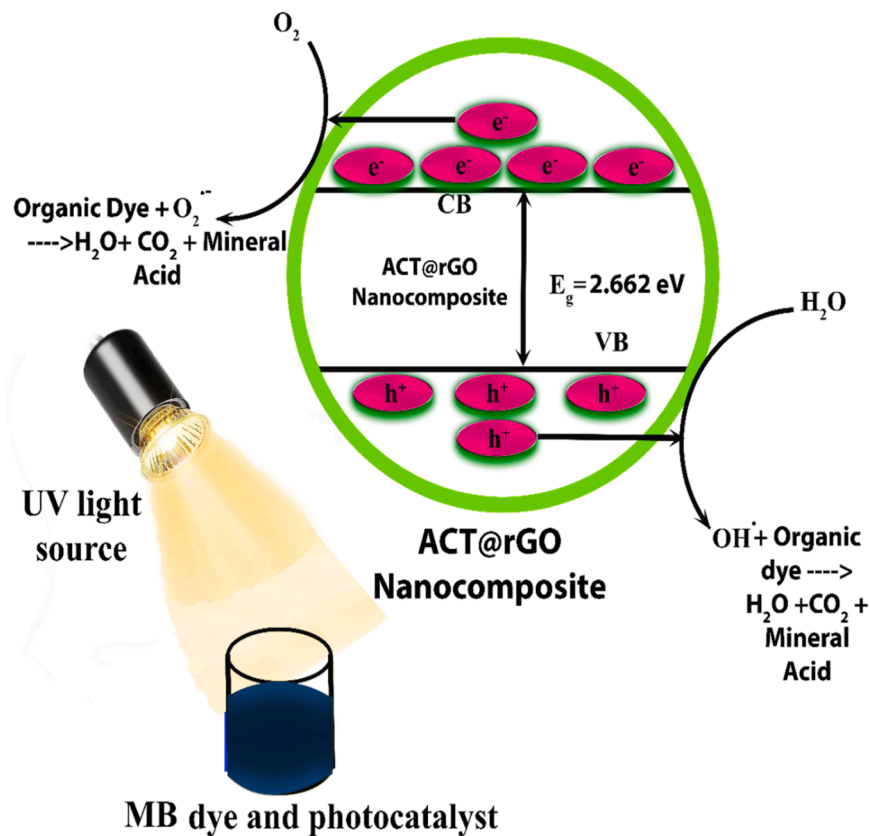
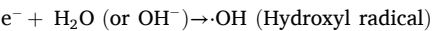


Fig. 13. MB dye degradation mechanism of ACT@rGO NCs.



Hydroxyl radical production:
Various electrons may combine with H_2O or OH^- to produce very reactive $\cdot OH$ radicals, which might assist in break down organic materials:



Overall photocatalytic reaction
A possible method to show the whole photocatalytic breakdown of MB is as follows:
 $Al_2O_3-CuO-TiO_2-rGO + h\nu + \text{Methylene Blue dye} + H_2O \rightarrow \text{Dye degraded products} + \cdot OH + O_2$.

4.4. ACT@rGO NCs: Anticorrosive study

The corrosion inhibition characteristics of ACT@rGO NCs were conducted at room temperature against MS in a 1.0 N H_2SO_4 solution used as a corroding medium. Weight loss (mg) and the rate of corrosion were noted under identical environmental conditions with and without rGO-based NCs.

Table 1
Weight loss corrosion data for MS samples in the presence of different concentrations of NCs after 13 h of exposure in 1.0 N H_2SO_4 .

Concentration (ppm) of rGO-based NCs	Weight loss (mg)	Corrosion rate (mpy)	Inhibition efficiency (%)
10	9.5	73.64	99.07
20	14.7	113.95	98.57
50	42.3	327.89	95.90
70	24.9	193.01	97.58
100	61.9	479.82	94.01
Blank	1032.3	8001.36	-

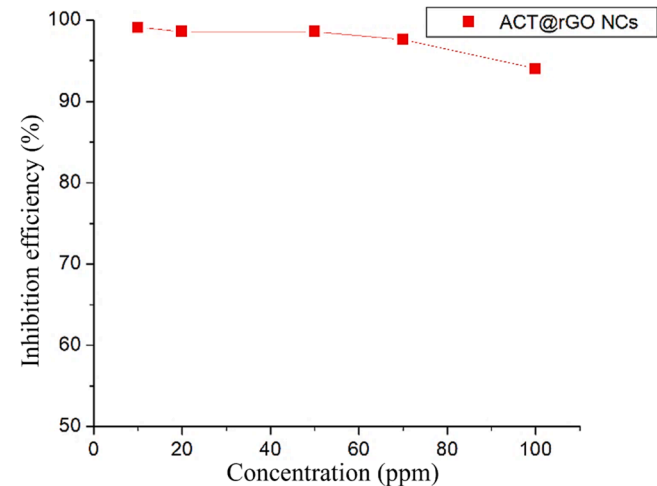


Fig. 14. Variation in CIE (%) versus concentration of ACT@rGO NCs at STP.

Corrosion rate was observed from Eq. (5) using standard ASTM procedure [81–83].

$$\text{Corrosion rate} = \frac{534 \times \text{Wt. loss}}{\text{Density} \times \text{Area} \times \text{Time}} \quad (5)$$

Inhibition efficiency was observed using Eq. (6).

$$\text{Inhibition efficiency (\%)} = \frac{CR_{Blank} - CR_{Inhibitor}}{CR_{Blank}} \times 100 \quad (6)$$

Table 1 shows weight loss data from corrosion experiments. Fig. 14 demonstrates the relationship between the concentration of NCs and CIE. The effectiveness of inhibition decreases as the concentration of

NCs increases. Sometimes product inhibition was observed in rGO-based NCs. CIE achieved a maximum of 99 % when the concentration of NCs was 10 ppm. One possible explanation for a decline in CIE as NC concentration rises might be the agglomeration of NCs particles at greater concentrations, which reduces the surface area accessible for MS contact.

There may be a saturation point beyond which increasing the concentration of the NCs does not lead to a proportional increase in the creation of the protective film on the MS surface [84]. Once the surface of MS is adequately covered, further additions of NCs may not significantly contribute to corrosion inhibition. The other probable reason for the decrease in CIE with the concentration of NCs is that excess NCs concentration may lead to the formation of undesirable by-products or compete with the desired corrosion inhibition process. This can diminish the overall effectiveness of corrosion inhibition [85].

5. DFT (computational) study of rGO NCs

A DFT research was conducted on rGO to identify reactive sites for adsorption and corrosion inhibition mechanisms demonstrated by rGO for MS alloys to support the experimental work. Kumar et al. conducted research of a similar nature. In an acidic solution, they looked at *Allium sativum L* as a green corrosion inhibitor for MS. The adsorption of green inhibitors on Mild steel surfaces is supported by both theoretical and experimental research [86]. Gaussian09W was used to carry out the first geometry optimization experiments. The geometry-optimized rGO was used for the energy and frequency investigation. The geometry-optimized structure of rGO is displayed in Fig. 15.

Fig. 16 represents the lowest unoccupied and highest occupied molecular orbitals (HOMO and LUMO) of rGO. The red region in Figs. 15–17 shows the area that has a greater electron density (ED), whereas the green color indicates the area that has a small ED. The orange color zone represents the area with intermediate ED [87].

A contour map Obtained from a Density Functional Theory (DFT) study of a molecule such as rGO gives an understanding of various chemical properties (Fig. 17). DFT is a computational approach based on quantum mechanics which is used to determine the electronic configuration of molecules [88]. Contour maps illustrate various features on a molecule's surface including spatial arrangement of electron density

surrounding the rGO.

The study of rGO using DFT entails knowledge of the atomic and molecular-level electronic structure and bonding [89]. However, the results that are achieved might vary depending on whether a hybrid function like B3LYP or an exchange-correlation function like Generalized Gradient Approximation (GGA) is used.

With the use of extensive data on the electronic band structure, electronic properties, band structures, band gaps, and the distribution of electronic states, and Density of States (DOS) of the rGO were calculated. To find out the conductivity of the rGO, the Fermi level location was computed.

A Bader charge analysis study was carried out to evaluate the distribution of charges within the rGO. The theoretical parameters for rGO were calculated using Eqs. (7)–(14) [90,91].

$$\text{Hardness (global), } \eta = \frac{(I - A)}{2} \quad (7)$$

$$\text{Softness (global), } \sigma = \frac{1}{\eta} = \frac{2}{(I - A)} \quad (8)$$

$$\text{Electrochemical Potential, } \chi = \frac{(I + A)}{2} \quad (9)$$

$$\text{Fraction of e}^- \text{ transferred, } \Delta N = \frac{(\chi_{Fe} - \chi_{Inh})}{2 \times (\eta_{Fe} - \eta_{Inh})} \quad (10)$$

$$\text{Adsorption energy, } E_{Ad} = \frac{E_{s-x} - (E_s + E_x)}{n} \quad (11)$$

$$\text{Work function, } \Delta\phi = \frac{(\phi_{Fe} - \chi_{Inh})^2}{4(\eta_{Fe} + \eta_{Inh})} \quad (12)$$

$$\text{Electron accepting power, } \omega^- = \frac{(3I + A^2)}{(16(I - A))} \quad (13)$$

$$\text{Electron releasing power, } \omega^+ = \frac{(I + 3A^2)}{16(I - A)} \quad (14)$$

We compared computational data produced with DFT by experimental results to validate the theoretical conclusions. The geometry-optimized structure is displayed in Fig. 15. rGO's HOMO (A) and LUMO (B) are shown in Fig. 16. The contour map of the HOMO (A) and LUMO (B) of rGO are shown in Fig. 17. 2.87 eV was the observed theoretical band gap. A little discrepancy in the band gap between the DFT and UV-visible research is readily apparent due to the varying ecological circumstances between these two methodologies. It was discovered to be similar to the band gap discovered in the UV-visible study's Tauc plots.

In Figs. 15–17, the area of high ED is shown by the red section, while the area of low ED is represented by the green color. The region of intermediate ED is shown by the orange color. It was discovered that the values of global hardness (η) and electrochemical potential (μ) were 1.43 and 7.77, respectively. The rGO's electrophilicity character (61.03) and global softness (σ) were 0.69 and 0.69, respectively. It was discovered that the charge transfer maximum (ΔN) was 3.01. Table 2 indicates that the electron-donating capacity of rGO is somewhat greater than its electron-accepting property.

A molecule's or material's polarizability is gauged by its global softness. It measures the degree to which a system's electron density can adapt to variations in the outside world. High softness denotes a system's propensity to give electrons and ease of polarization. Due to its significantly lower softness (0.69), rGO is tough to polarize and has a propensity to absorb electrons rather than donate them. rGO has a global hardness of 1.43, which suggests that it has electrophilic properties. Higher hardness materials are often less reactive to chemicals and less prone to charge transfer, making them more stable.

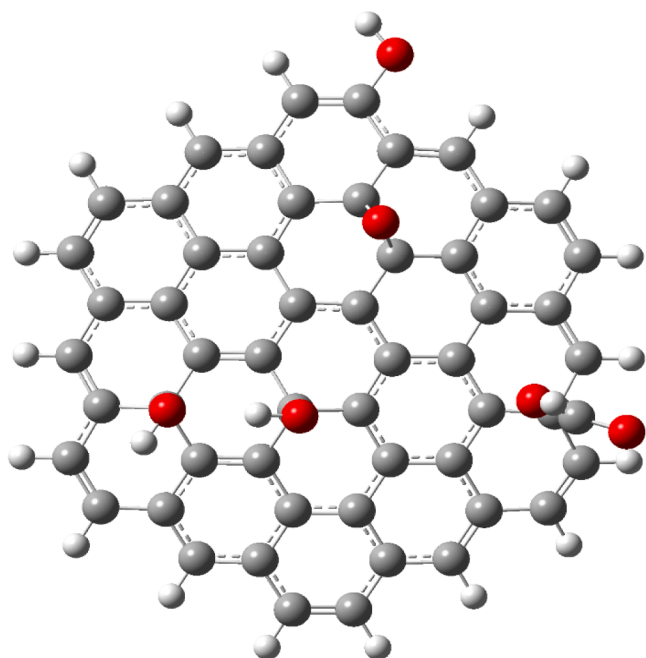


Fig. 15. Geometry optimized structure of rGO.

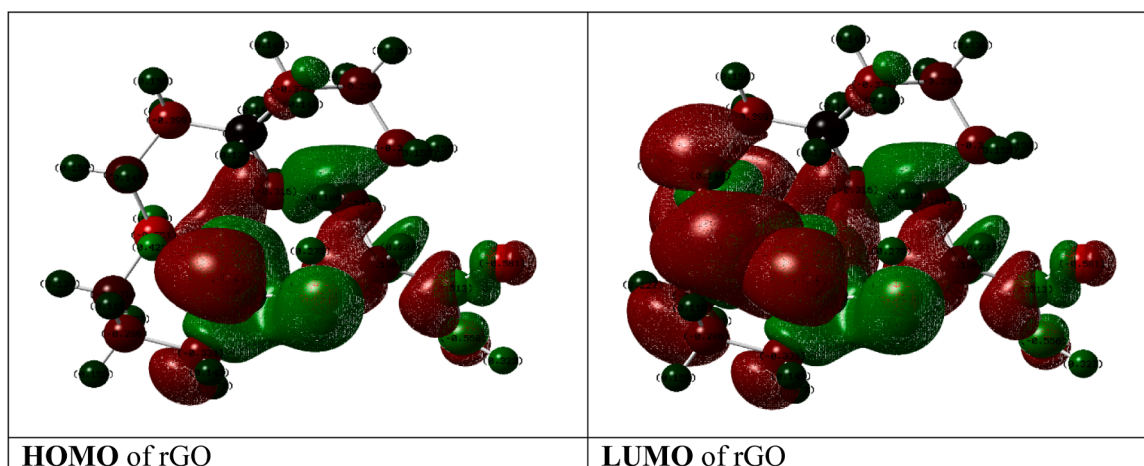


Fig. 16. HOMO and LUMO molecular orbitals of rGO NCs.

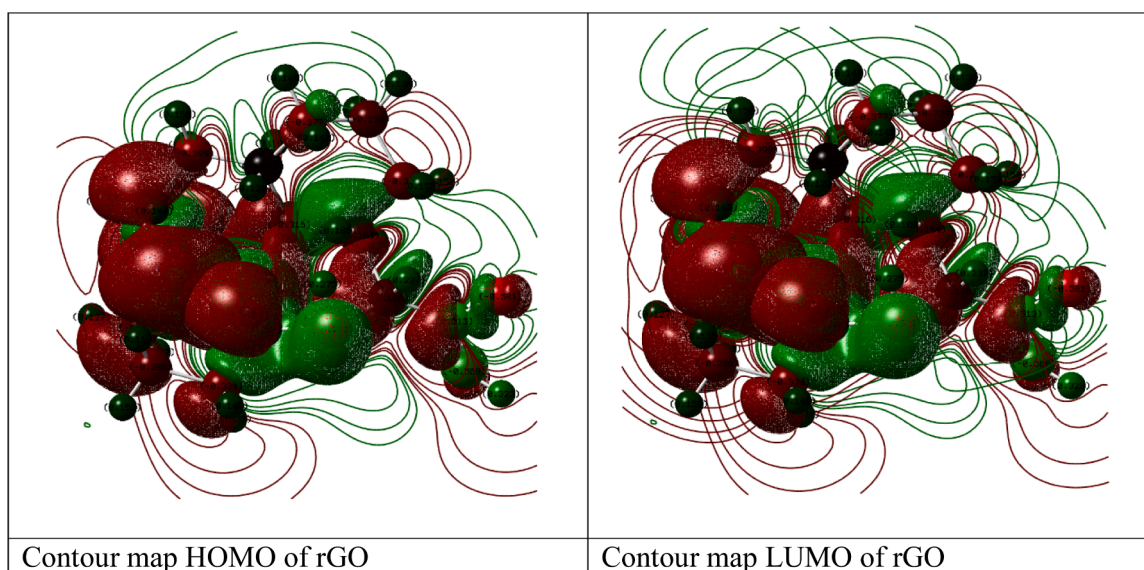


Fig. 17. Contour map of rGO NCs.

Table 2

DFT parameters of rGO NCs (Basis set): 6-31G(d), (6D, 7F) acquired from in silico study.

E_{HOMO} (-eV)	E_{LUMO} (-eV)	ΔE (eV)	I (eV)	A (eV)	χ (eV)	η (eV)	σ (eV ⁻¹)
6.34	9.21	2.87	6.34	9.21	7.77	1.43	0.69
ΔN (eV)		ω (au)	ω^+ (au)	ω^- (au)			
2.71		61.03	2.47	1.86			

A conceivable method for the adsorption of rGO matrix on the MS iron atom surface is depicted in Fig. 18. Attacking sites are accessible nucleophilic sites on the surface of rGO. A single pair of electrons in the nitrogen atom and the unoccupied d-orbitals of the iron atoms combine to create a coordinate covalent connection. It is also feasible for iron atoms in their filled d-orbitals to donate back to nitrogen atoms in their unfilled antibonding orbitals. The ligand-to-metal and metal-to-ligand bonding that occurs forward and backward strengthens the adsorption of NCs on the MS surface.

6. Conclusions

We have achieved significant achievements in areas of materials science and nanotechnology with the study of the distinctive ACT@rGO NCs, that exhibits great potential in an array of applications. The addition of rGO has greatly enhanced the magnetic properties, antibacterial properties on Gram-positive and Gram-negative bacterial strains, photocatalytic efficacy, and anticorrosive properties of ACT NPs. In the environmental purification field, our research has revealed the remarkable photocatalytic capability of these NCs, as evidenced by the MB dye degradation in UV (94.7 %) and visible light (70.5 %). Furthermore, their effectiveness in protecting critical infrastructure is demonstrated by their excellent CIE against MS in an acidic medium (99.07 % at 10 ppm concentration).

When exposed to UV light, the NCs exhibit strong photocatalytic activity against MB dye. In 1.0 N H₂SO₄ solution, the NCs exhibit anti-corrosive properties (CIE of 99 %) against MS. A paramagnetic property ($\chi = 0.14$) is seen in the NCs. Zone of inhibition against strains of *S. aureus* and *E. coli* bacteria demonstrates their potential as a weapon to fight against microbial infection. Comparing the zone of inhibition (mm) with that of Ampicillin, a common antibiotic, revealed that NCs show almost similar ZoI. The theoretical (DFT) investigation and the

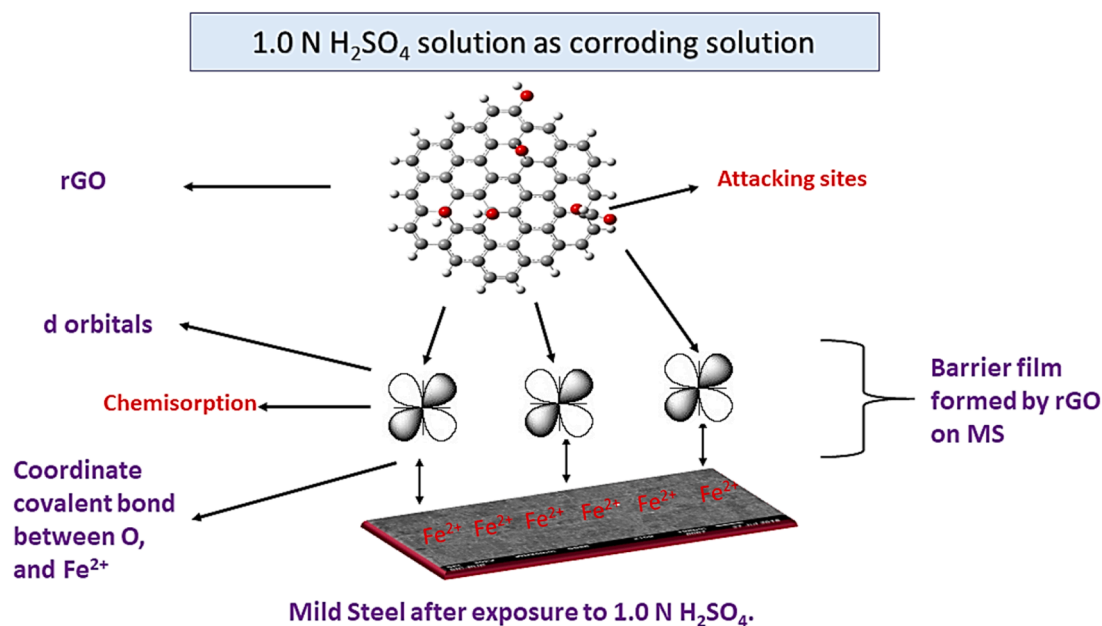


Fig. 18. Plausible mechanism of adsorption rGO on the mild steel surface.

experimental findings augment each other results. The cutting-edge ACT@rGO NCs provide novel approaches to a variety of complex problems, therefore bringing about a paradigm change in materials research. Their flexibility is shown by their ability to handle problems related to environmental cleanup, corrosion prevention, biomedical technology, and water purification, all at the same time. These NCs have a promise for real-world use, helping to create a more technologically sophisticated, healthier, and environmentally friendly world.

Potential challenges, limitations, and avenues for future research

This research article highlights several promising aspects of ACT@rGO NCs across different fields including materials science, nanotechnology, environmental remediation, biomedical applications, and corrosion prevention. However, certain potential challenges, limitations, and avenues for future research could be explored. While the study demonstrates promising results at the laboratory scale, scaling up the production of ACT@rGO NCs for practical applications may present challenges. Ensuring consistent quality and reproducibility of the NCs on a larger scale will be essential for their widespread adoption. The durability and stability of ACT@rGO NCs under real-world conditions, such as exposure to harsh environments or prolonged use, need to be thoroughly investigated. The photocatalytic property of ACT@rGO NCs for organic dye degradation is demonstrated, and further optimization of the photocatalytic performance, such as enhancing the efficiency under visible light or extending the range of target pollutants, could expand their applicability in environmental remediation. The biocompatibility and potential toxicity of ACT@rGO NCs need to be thoroughly evaluated in biomedical applications. While the study provides experimental evidence of the enhanced properties of ACT@rGO NCs, further mechanistic insights into the underlying processes, such as the role of graphene oxide in improving magnetic properties, antimicrobial activity, corrosion resistance, and photocatalytic efficacy, could provide valuable information for optimizing the design of these NCs. Assessing the cost-effectiveness and sustainability of producing ACT@rGO NCs on a large scale will be critical for their commercial viability. Addressing these challenges and exploring avenues for further research will be essential for realizing the full potential of ACT@rGO NCs in addressing multifaceted challenges in various fields and fostering technological advancements toward a greener and healthier future.

Declaration of use of AI tools

We certify that, in authoring this research study, we did not use any artificial intelligence (AI) tools.

CRediT authorship contribution statement

Rahul Sharma: Writing – original draft, Methodology, Conceptualization. **Harish Kumar:** Writing – review & editing, Visualization, Validation, Supervision, Investigation, Conceptualization. **Chetna Saini:** Visualization, Validation. **Diksha Yadav:** Visualization, Validation. **Kajal Yadav:** Visualization, Validation. **Saloni:** Visualization, Validation. **Minakshi:** Validation, Investigation. **Antresh Kumar:** Validation, Methodology. **Gita Rani:** Visualization, Validation.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Harish Kumar reports administrative support was provided by Central University of Haryana. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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