Application Driven Design: Harnessing Titanium Carbide Bismuth Phosphate Nanocomposites for Advanced Antimicrobial Materials

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**Abstract:** The lack of intrinsic antibacterial characteristics of polymer/layered silicate nanocomposites poses a challenge for their usage in food packaging, medical devices, and industrial applications. By adding antibacterial activity, these materials' application potential may be greatly increased, improving food safety, health outcomes, and product longevity. This work investigates the synthesis and characterisation of Ti3C2/BiPO4 nanocomposites, which combine the antibacterial and photocatalytic qualities of bismuth phosphate with the mechanical strength and conductivity of titanium carbide. Bismuth phosphate is made by chemical precipitation, titanium carbide is made by HF etching, and then the particles are reduced by microwave method. X-ray diffraction (XRD), transmission electron microscopy (TEM), high-resolution TEM (HR-TEM), Fourier-transform infrared spectroscopy (FTIR), selected area electron diffraction (SAED), and UV-visible diffuse reflectance spectroscopy (UV-Vis DRS) are some of the technologies used for characterization.When it comes to Aspergillus niger and Candida albicans, the nanocomposites show strong antibacterial action. Practical uses need addressing challenges such biocompatibility, regulatory problems, and complexity of synthesis. To fully exploit the promise of Ti3C2/BiPO4 nanocomposites in a variety of applications, future research should concentrate on refining synthesis techniques, conducting extensive biocompatibility evaluations, and investigating new functions.

**keywords:** Antimicrobial nanocomposites, Pseudocapacitors, antibacterial activity, multidisciplinary approach, particular enzymes, oxoacid salt photocatalyst

# Introduction

Although a wide range of polymer/layered silicate nanocomposite goods are available on the market, including dental materials, food packaging films, containers, and engine parts, their application potential is restricted due to their lack of intrinsic antibacterial qualities. By adding antibacterial activity, these nanocomposites could become much more useful and have a wider range of applications. Antimicrobial nanocomposites, for example, can increase food safety and shelf life in food packaging by reducing microbial contamination. These materials have the potential to enhance patient outcomes and lower the risk of infections in medical and dental applications. Likewise, the presence of antibacterial qualities in industrial and engine components may lead to more durable and hygienic products. Consequently, creating polymer/layered silicate nanocomposites with antibacterial activity is a critical first step in discovering new, worthwhile applications.[(Amrane et al. 2020; Raneesh et al. 2018; Bauccio 1993)](https://paperpile.com/c/AdPeJv/5uJL+q1ME+wWTz)

Application-driven design in the context of Ti3C2/BiPO4 nanocomposites for improved antimicrobial materials entails modifying these nanocomposites' characteristics and capabilities to satisfy particular application needs. Using a multidisciplinary approach, this process combines materials science to comprehend and control the mechanical and structural properties; nanotechnology to precisely control the characteristics of the nanoparticles; chemistry to synthesize and modify the composites for enhanced activity and stability; biology to comprehend and optimize interactions with microbes; and engineering to integrate the materials into real-world applications, guaranteeing scalability and manufacturability. Researchers can develop extremely useful and effective antimicrobial materials for a variety of applications, including food packaging, medical devices, and filtration systems, by utilizing knowledge from these domains..[(Suhir 1991)](https://paperpile.com/c/AdPeJv/wvx8)[(Tahir 2023; Twardowski 2007)](https://paperpile.com/c/AdPeJv/Ezh3+Es7v)

Furthermore, in order to meet particular application needs, the Ti3C2/BiPO4 nanocomposites may be designed with extra functions. When photothermal or photodynamic capabilities are integrated, for example, the nanocomposites can demonstrate light-triggered antimicrobial activity, in which exposure to light causes localized heating or the formation of reactive oxygen species, which efficiently kills bacteria. Furthermore, the addition of stimulus-responsive components can enable the antimicrobial agents to release on demand in response to environmental stimuli like pH, temperature, or the presence of particular enzymes. By ensuring that the antimicrobial chemicals are only released when necessary, this strategy improves efficiency and lowers the possibility of resistance developing.By incorporating these cutting-edge features, the nanocomposites can be precisely adjusted to function at their best in a range of situations, from medical coatings that react to infection indicators to smart packaging that activates when contamination is detected, thus increasing their usefulness and practicality.[(Redmond et al. 1957; Das, Rosenkranz, and Ganguly 2023; Darroudi et al. 2023)](https://paperpile.com/c/AdPeJv/XItS+qeUq+eA8G)

Extensive characterisation and testing are necessary throughout the design phase to verify the Ti3C2/BiPO4 nanocomposites' performance for the intended use. This might involve testing mechanical and chemical stability under appropriate circumstances, evaluating biocompatibility through in vitro and in vivo research, and determining the effectiveness of antibiotics using established testing procedures.[(Denizli and Saylan 2021)](https://paperpile.com/c/AdPeJv/3oiU). Modern society's growing needs combined with growing ecological concerns have created a need for innovative, affordable, eco-friendly, and high-performing energy storage solutions. Supercapacitors (SCs) and ultracapacitors, other names for electrochemical capacitors (ECs), have attracted a lot of interest as energy-storage devices because of their high power density, quick charge-discharge speed, good reversibility, and extended cycle life. Pseudocapacitors and electrical double-layer capacitors (EDLCs) are the two charge storage devices that power ECs. Activated carbon, carbon nanotubes, and graphene-based materials are examples of porous carbon electrodes on which ions can electrosorb to store charge in EDLCs. Conversely, pseudocapacitors have higher energy densities but usually have shorter cyclic lives since they rely on redox processes to hold charge. Conductive polymers and transition metal oxides are common materials used in pseudocapacitors.[(Ma et al. 2021; Deutsch 1949; Redmond et al. 1957)](https://paperpile.com/c/AdPeJv/3oYZ+GyJe+XItS)

## Bismuth Phosphate

Because of its remarkable optical qualities, non-toxicity, cheap cost, and high catalytic efficiency, bismuth phosphate (BiPO4), an oxoacid salt photocatalyst, has promise in ion sensing, radioactive element separation, and catalysis. Research has shown that under UV light, BiPO4 demonstrates notable photocatalytic oxidative capabilities for breaking down organic pigments. Furthermore, studies indicate that the nonmetal oxy-acid PO43− facilitates photoinduced electron–hole pair separation. The present BiPO4 photocatalytic system has drawbacks despite these benefits, such as weak adsorptive performance, big particle size, and quick recombination of photoinduced electron-hole pairs. Numerous methods, including ion doping, surface modification with noble metals, and coupling with other semiconductors, have been suggested to increase the photocatalytic activity of BiPO4.[(Stephan 1949; Kumar 2024; Korotcenkov 2020)](https://paperpile.com/c/AdPeJv/hxmn+wgHo+aFxx)

## Characteristics of TitaniumCarbide Bismuth Phosphate

First and foremost, it's critical to comprehend the special qualities of Ti3C2/BiPO4 nanocomposites. Ti3C2, or titanium carbide, is a two-dimensional nanomaterial from the MXenes family that has a high mechanical strength, conductivity, and surface area. Conversely, BiPO4 is a bismuth-based substance well-known for its antibacterial qualities. Synergistic effects can be obtained by mixing these elements into nanocomposites, which will enhance antibacterial activity while preserving other desired features.

The next step is to determine the particular application requirements. Considerations including biocompatibility, stability in biological contexts, and tailored antibacterial action against clinically relevant infections, for example, are critical if the application is in a medical setting. Conversely, when the use is in consumer goods like fabrics or packaging materials, factors like robustness, ease of washing, and suitability for production methods become crucial.[(Deutsch 1949; Redmond et al. 1957; Kahlenberg 1912; Wakaki, Shibuya, and Kudo 2018)](https://paperpile.com/c/AdPeJv/GyJe+XItS+VSgK+vl04)

## Antimicrobial properties of Titanium Carbide Bismuth Phosphate

The capacity of polymer/layered silicate nanocomposites to combine the structural, physical, and chemical features of both inorganic and organic materials has attracted a lot of attention in recent years. Rectorite (REC) may have benefits, even though montmorillonite (MMT) has received the majority of study attention. With a regular interstratified structure made up of alternating dioctahedral mica-like (nonexpansible) and dioctahedral montmorillonite-like (expansible) layers in a 1:1 ratio, REC is a layered silicate that shares properties with montmorillonite. Compared to normal montmorillonite, REC has bigger separable layer thickness and layer aspect ratio (area-to-thickness), which may improve the efficacy of nanolayer reinforcement in different characteristics and promote the production of intercalated or exfoliated nanocomposites.[(X. Wang et al. 2016; Khalid, Arshid, and Grace 2020; Cao and Wang 2011)](https://paperpile.com/c/AdPeJv/WNXy+P1O2+vgx7)

Although a wide range of polymer/layered silicate nanocomposite products, including food packaging films, containers, engine parts, and dental materials, are available on the market, there is a noticeable lack of these materials' antimicrobial activity, which would greatly expand their applications. Compounds like Titanium Carbide and Bismuth Phosphate are combined and new compound is produced with developed antimicrobial properties on their nanocomposites are found in an combined manner.[(Pillai and Lang 2021; Köhler and Fritzsche 2008; Inamuddin et al. 2020)](https://paperpile.com/c/AdPeJv/xVdQ+aR4l+fiuu)

# MATERIALS AND METHODS

To synthesize Bismuth Phosphate, begin by dissolving 2.9109 grams of Bismuth in 46 mL of distilled water, leading to the formation of sediments. To dissolve these sediments, add 4 mL of nitric acid and stir for 45 minutes at room temperature, creating solution A. Separately, dissolve 2.2713 grams of Disodium hydrogen phosphate in 50 mL of water to prepare the phosphate solution. Combine equal ratios of the Bismuth and Phosphate solutions to form solution B. Slowly add solution B to solution A while continuously stirring for 1 hour, resulting in solution C. The resulting Bismuth Phosphate precipitate will be white.

For synthesizing Titanium Carbide, mix Titanium Aluminium Carbide (Ti3AlC2) with 20 mL of hydrofluoric acid (HF). The aluminum component is etched by stirring the mixture with a pellet for 24 hours at 40°C. This temperature aids in removing the aluminum layer. Adjust the pH to 7, then centrifuge the compound and wash it with water until the pH stabilizes at 7, producing a green color. The precipitate is obtained and dried in a hot air oven at 80°C for 24 hours.

Using the microwave technique, the particles undergo a reduction process to form nanoparticles within 10 minutes—2 minutes for preparation and 5 minutes for the reduction process. To prevent contamination, subject the resulting mixture to centrifugation.

## Centrifugation involves the following steps

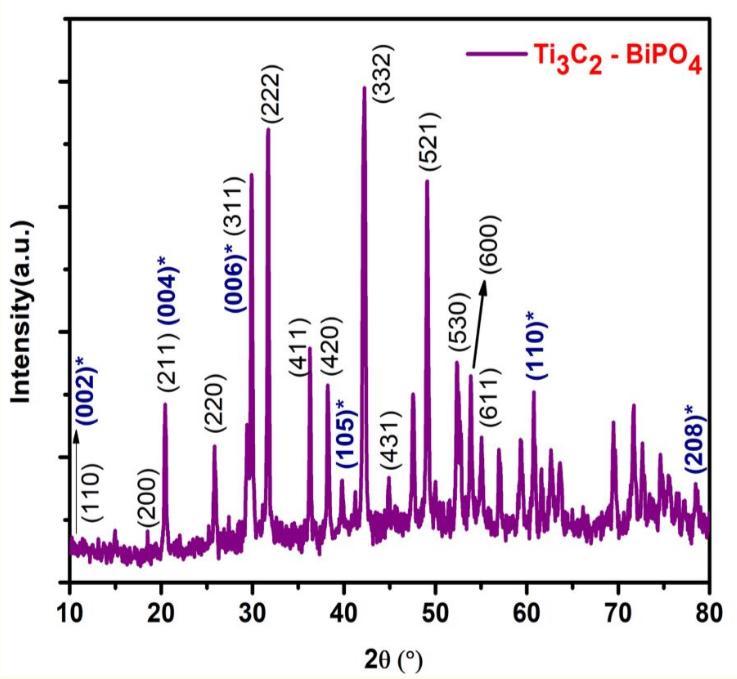
1. Centrifuge the mixture three times using distilled water.

2. Perform two rounds of centrifugation with ethanol.

3. Conduct two additional rounds of centrifugation using acetone.

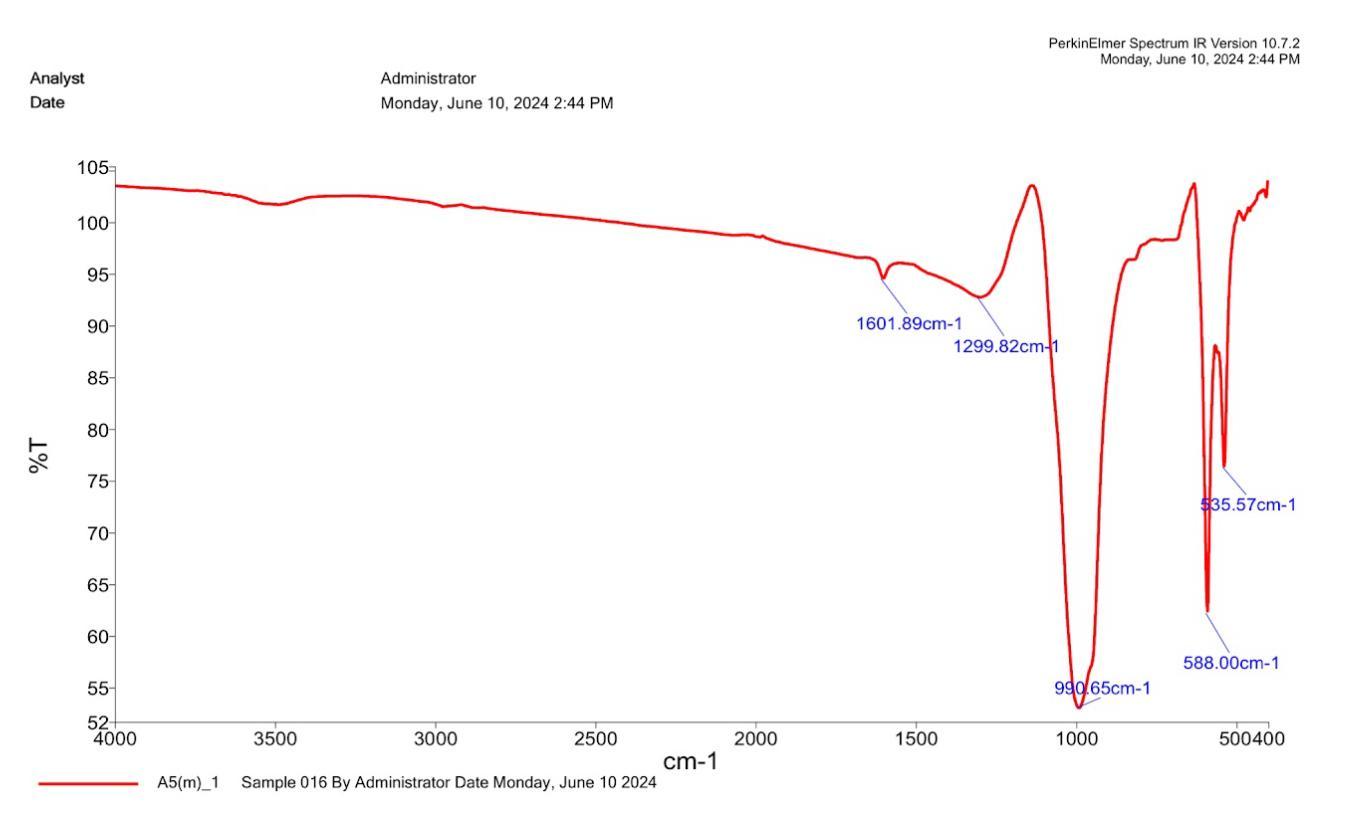
In total, the mixture undergoes seven rounds of centrifugation. After each centrifugation, remove the precipitate and dry it in a hot air oven at 80°C for 24 hours. Finally, carry out the calcination process for three hours at 300°C.

# RESULTS AND DISCUSSION

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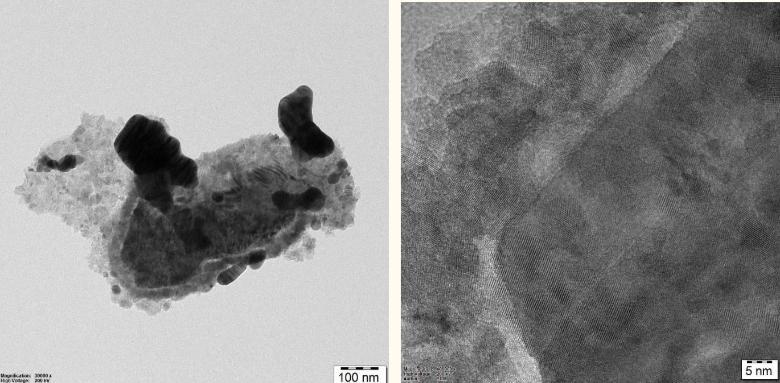
**Figure 1:** XRD patterns of Titanium Carbide Bismuth Phosphate nanoparticles

The X-ray diffraction (XRD) graph presented here details the analysis of Ti3C2-BiPO4, a material composed of titanium carbide (Ti3C2) and bismuth phosphate (BiPO4). XRD is utilized to investigate the atomic structure of crystalline substances by measuring how X-rays scatter off their crystal lattice planes. The graph's x-axis is labeled "20 (°)", indicating the 2 theta angle, a standard in XRD experiments that signifies the angle of X-ray diffraction[(Gogotsi and Simon 2011)](https://paperpile.com/c/AdPeJv/UZJ3). On the y-axis, labeled "Intensity (a.u.)", arbitrary units measure the intensity of diffracted X-rays, with taller blue lines indicating higher intensity peaks. These peaks correspond to the specific angles at which X-rays are scattered by the crystal lattice of Ti3C2-BiPO4. Throughout the graph, asterisks denote smaller bumps, each representing the intensity of X-rays diffracted by distinct crystal planes within the material, typically identified using Miller indices (e.g., (002)\*). Such analysis provides valuable insights into the material's crystalline structure, aiding in identifying its composition and atomic arrangement. Overall, the XRD experiment on Ti3C2-BiPO4 seeks to elucidate its crystallographic properties and potentially guide its applications in various fields, from materials science to catalysis and beyond.These peaks correspond to the specific angles at which X-rays are scattered by the crystal lattice of Ti3C2-BiPO4[(Darroudi et al. 2023)](https://paperpile.com/c/AdPeJv/eA8G). Throughout the graph, asterisks denote smaller bumps, each representing the intensity of X-rays diffracted by distinct crystal planes within the material, typically identified using Miller indices (e.g., (002)\*). Such analysis provides valuable insights into the material’s crystalline structure, aiding in identifying its composition and atomic arrangement[(Darroudi et al. 2023; Torres 2012)](https://paperpile.com/c/AdPeJv/eA8G+18Ia). Overall, the XRD experiment on Ti3C2-BiPO4 seeks to elucidate its crystallographic properties and potentially guide its applications in various fields, from materials science to catalysis and beyond.



**Figure 2:** FTIR spectrum of Titanium Carbide Bismuth Phosphate nanoparticles

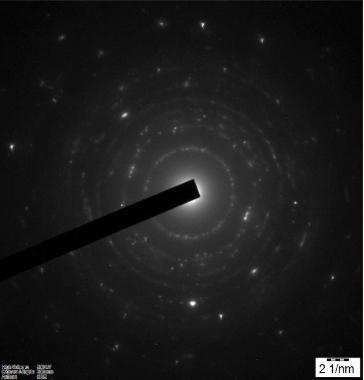
An infrared (IR) spectrum is a vital analytical technique for identifying and evaluating chemical compounds through the study of their molecular vibrations, and this graph is one example of one. In IR spectroscopy, the wavenumber is commonly measured in reciprocal centimeters (cm⁻¹), with a range of 4000 to 400 cm⁻¹. This measurement is inversely correlated with wavelength. The transmittance percentage (%T) on the y-axis represents the quantity of infrared light that passes through the sample; more absorption at particular wavenumbers is correlated with lower transmittance[(Torres 2012)](https://paperpile.com/c/AdPeJv/18Ia). The different vibrational modes of the molecules in the sample give rise to peaks on the spectrum. For example, the peak at 1601.89 cm⁻¹ most likely represents C=C stretching vibrations, which are indicative of double bonds in alkenes or aromatic rings. The peak at 1299.82 cm⁻¹ could represent C-N stretching vibrations, which are frequently seen in amides and amines and indicate the existence of functional groups that include nitrogen[(Friedrich and Schlarb 2011)](https://paperpile.com/c/AdPeJv/AKKz). The peak at 990.65 cm⁻¹ may represent aromatic rings or double bonds by way of C=C bending in alkenes or out-of-plane bending vibrations of aromatic C-H bonds. The peak at 435.57 cm⁻¹ may be linked to skeletal vibrations, which are frequently observed in the fingerprint region of the infrared spectrum and contain distinct vibrational patterns for various molecules. In a similar vein, the peak at 588.00 cm⁻¹ may represent out-of-plane bending vibrations, which are also frequent in aromatic compounds[(Tahir 2023)](https://paperpile.com/c/AdPeJv/Ezh3). Chemists can determine which functional groups are present in a chemical and deduce its molecular structure by closely examining these peaks.This in-depth analysis frequently entails contrasting the measured spectrum with reference spectra from reputable databases, which enables the identification of the molecule by comparing its distinct vibrational signature with samples that are known to exist. For molecular identification and structural study, IR spectroscopy offers a non-destructive and highly informative technique that is crucial in many domains, including organic chemistry, medicines, and materials research.[(Tahir 2023; Zhao et al. 2023)](https://paperpile.com/c/AdPeJv/Ezh3+a4Yd)



1. **(b)**

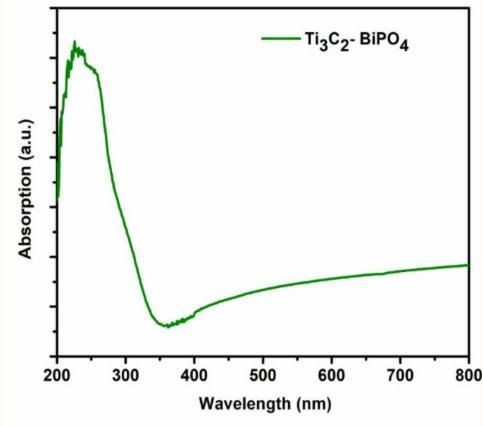
**Figure 3** (a,b):TEM and HRTEM images of Titanium Carbide Bismuth Phosphate nanoparticles

The photos that are offered are from High-Resolution Transmission Electron Microscopy (HR-TEM) and Transmission Electron Microscopy (TEM), which are used to examine the morphological and structural characteristics of nanomaterials. With a 100 nm scale bar, the TEM picture on the left shows a cluster of nanoparticles at a lower magnification, providing a general overview of the distribution and shape of the particles.[(Tahir 2023; Zhao et al. 2023; C. Wang et al. 2014)](https://paperpile.com/c/AdPeJv/Ezh3+a4Yd+jq9h) Whereas lighter portions indicate thinner areas or lower electron density, darker sections show higher electron density, which is suggestive of heavier components or thicker areas. This picture shows that the nanoparticles have a tendency to group together. Their sizes are typically in the nanometer range, and some of them have unique forms that might be indicative of crystallinity.It displays lattice fringes, which are indicative of crystalline materials and aid in determining lattice spacing[(Zhou, Dong, and Jin 2018)](https://paperpile.com/c/AdPeJv/CMAY). These fringes correspond to atomic planes inside the crystal structure. The regularity and direction of the lattice fringes provide information about the crystallographic quality, and their presence verifies the nanoparticles' crystalline origin. Any perturbations in these fringes may point to amorphous areas or flaws.[(Raneesh and Visakh 2021)](https://paperpile.com/c/AdPeJv/hC80) These photos collectively imply that the substance is made up of crystalline nanoparticles that group together to form clusters. Potential uses in domains where particle size and crystallinity are crucial, such as materials science, electronics, or catalysis, are suggested by this crystalline structure(Rafi et al., 2024). Additional investigations, such Selected Area Electron Diffraction (SAED) for precise crystallographic information or Energy-Dispersive X-ray Spectroscopy (EDS) for elemental composition, may be carried out in order to gain a deeper understanding of the material.All things considered, these TEM and HR-TEM pictures offer vital details on the size, form, and crystalline makeup of the nanoparticles, which are critical for evaluating their possible uses and effectiveness in a range of technical domains.[(Raneesh and Visakh 2021; Thomas et al. 2017)](https://paperpile.com/c/AdPeJv/hC80+gq5u)



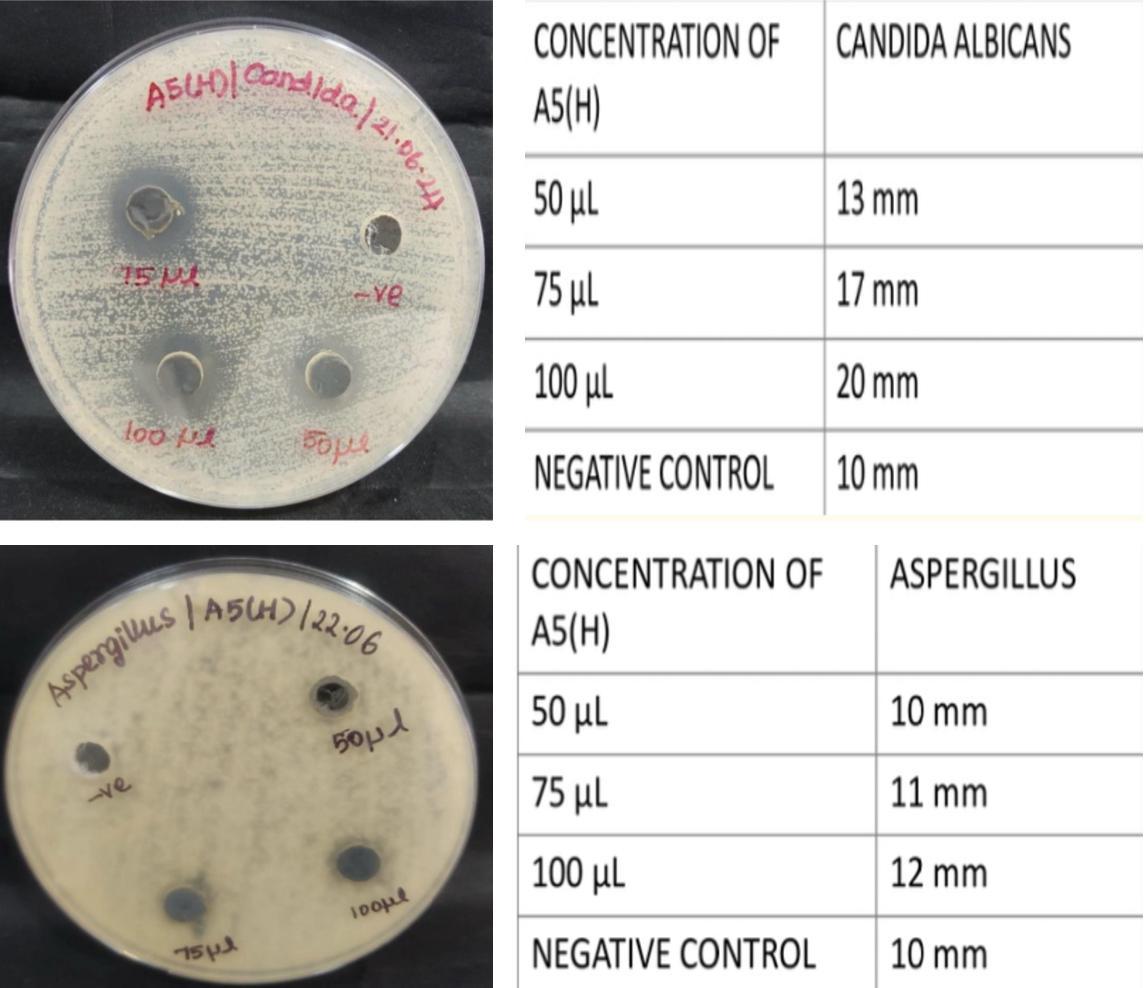
**Figure 4:** Selected Area Diffraction patterns of Titanium Carbide and Bismuth Phosphate nanoparticles.

Although "Ti₃C₂-BiPO₄" is mentioned in the subject, which corresponds with the picture content, Selected Area Electron Diffraction (SAED) image interpretation necessitates specific crystallographic expertise. SAED pictures show how electrons diffract off the crystal lattice of a material, providing important details regarding the arrangement of atoms.[(Liu et al. 2018)](https://paperpile.com/c/AdPeJv/88dw) Scientists require in-depth understanding of the material's crystal structure, orientation beneath the electron beam, and particular experimental circumstances in order to interpret an SAED picture with accuracy (Tuluwengjiang et al., 2024). Usually, these pictures display a pattern of rings or dots, each of which represents a distinct crystallographic plane.The diffraction from crystalline areas is characterized by the whirling black and white pattern observed in SAED pictures[(Huang et al. 2022)](https://paperpile.com/c/AdPeJv/NrSC). Understanding the diffraction pattern for Ti₃C₂-BiPO₄ can aid in determining crystallite size, phase purity, and any flaws or strain inside the crystal. Still, a definite interpretation is difficult to come by without precise parameters like the zone axis, camera length, and indexing of diffraction spots. These specifics are used by crystallography experts to compare actual patterns with theoretical expectations, enabling accurate identification of the structure and orientation of crystals. As a result, although the overall characteristics of the SAED picture may be explained, a thorough crystallographic study and context-specific data are necessary for a full interpretation.[(Riazi et al. 2021)](https://paperpile.com/c/AdPeJv/xpF6)



**Figure 5:** UV and Visible spectra patterns of Titanium Carbide and Bismuth Phosphate nanoparticles

Ti3C2-BiPO4's absorption spectrum offers a thorough understanding of how light interacts with it throughout the electromagnetic spectrum. The graph shows the wavelength (X-axis in nanometers) vs absorption intensity (Y-axis) to show the different features of the material's light absorption. In the ultraviolet (UV) region, Ti3C2-BiPO4 shows prominent absorption peaks, suggesting substantial absorption of shorter wavelengths that correspond to higher energy photons. This implies that the material is capable of efficiently absorbing UV light, maybe as a result of electronic changes occurring in its crystalline or molecular structure.[(Raneesh and Visakh 2021)](https://paperpile.com/c/AdPeJv/hC80) On the other hand, the visible light spectrum exhibits less absorption, especially at longer wavelengths, suggesting that Ti3C2-BiPO4 may transmit more of these wavelengths. The precise hue of the substance cannot be ascertained only from the absorption spectrum, even while this indicates that it may look colored—likely as a result of its selective absorption in the UV and potentially shorter visible wavelengths[(Raneesh and Visakh 2021; Khan, Pradhan, and Sohn 2017)](https://paperpile.com/c/AdPeJv/hC80+5THY). To precisely determine Ti3C2-BiPO4's perceived color, further information would be required, such as reflectance spectra or colorimetric studies. However, the absorption spectrum demonstrates its optical characteristics and its uses as a filter material or for UV shielding when selective light absorption is advantageous.[(Raneesh and Visakh 2021; Khan, Pradhan, and Sohn 2017; Pomogailo and Kestelman 2006)](https://paperpile.com/c/AdPeJv/hC80+5THY+5Lit)



**Figure 6:** The antimicrobial effects of Titanium Carbide and Bismuth Phosphate nanoparticles against Candida Albicans and Aspergillus

The Ti3C2-bismuth phosphate nanocomposite's antifungal activity against Aspergillus niger and Candida albicans is visually assessed in this experiment.[(El-Gazzar et al. 2024)](https://paperpile.com/c/AdPeJv/Sd2j) Different portions with varying quantities of the nanocomposite material and fungus are displayed in each petri plate. Larger zones signify more powerful antifungal actions. Clear zones surrounding the material portions show locations where fungal growth is suppressed. In comparison to Aspergillus niger, a greater inhibition was seen surrounding Candida albicans sections, which may indicate a higher susceptibility of Candida albicans to the nanocomposite.[(Elsherbiny et al. 2024)](https://paperpile.com/c/AdPeJv/aXGa) However, further information is needed, such as the precise doses examined, control trials without the nanocomposite, and statistical analysis of inhibitory zones, in order to make firm judgments regarding the nanocomposite's overall performance. A number of other factors need to be taken into account, including the nanocomposite's practical usability in various situations, potential side effects on adjacent tissues or surroundings, and its method of action against fungus.[(Joshi 2020)](https://paperpile.com/c/AdPeJv/VOcS) To completely comprehend and evaluate the antifungal activities of the Ti3C2-bismuth phosphate nanocomposite and its potential as a therapeutic or preventative agent against fungal infections, further extensive investigation and testing are vital.[(Joshi 2020; Katta et al. 2024)](https://paperpile.com/c/AdPeJv/VOcS+iKrJ)

# CONCLUSION

Ti3C2/BiPO4 nanocomposites shows promise for antimicrobial application due to their combination of titanium carbide’s mechanical strength and conductivity with bismuth phosphate’s antibacterial and photocatalyticproperties. Despite their potential, challenges like complex synthesis, biocompatibility issues, environmental concerns, and regulatory requirements must be addressed for practical development. Future research should prioritize optimizing synthesis methods, conducting through biocompatibility assessments, and exploring advanced functionalities. Collaboration across disciplines and adherence to regulatory standards will be critical to realizing the full potential of Ti3C2/BiPO4 nanocomposites in real- world applications, ensuring both efficiency and safety in diverse settings from healthcare to food safety and beyond.Optimizing synthesis methods for scalability and cost-effectiveness is essential for economic viability. Ensuring consistent quality throughout production is vital for product reliability. Comprehensive studies are needed to assess biocompatibility and long-term safety, particularly for medical applications. These studies ensure materials are safe and do not cause adverse biological responses.

# LIMITATIONS

Ti3C2/BiPO4 nanocomposites have a complicated synthesis method that makes it difficult to maintain consistency and scalability for industrial manufacturing. Furthermore, careful research is needed to address toxicity and biocompatibility problems, particularly with regard to applications in the food and medical industries. Production is made more difficult by the rising cost of raw materials, which emphasizes the need for cost-effective strategies and improved synthesis techniques to overcome these obstacles and guarantee useful, secure, and profitable applications.

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