A Novel Antimicrobial Coating Composed of MXene-Chitosan on the Surface of Orthodontic Brackets

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Abstract

Background: Orthodontic treatment can create favorable environments for bacterial growth, increasing the risk of demineralization and oral infections. MXene-based materials are known for their excellent antimicrobial and biocompatibility properties. **Aim:** This study investigates the antimicrobial properties and biocompatibility of a novel MXene-Chitosan coating on orthodontic brackets. **Materials and Methods:** Ti3C2Tx MXene was synthesized and dispersed in deionized water. Chitosan solution (1%) was prepared and mixed with MXene at a 1:1 ratio. Orthodontic brackets were cleaned, sterilized, and dip-coated in the MXene-Chitosan solution. The antimicrobial activity was assessed using agar diffusion against *Streptococcus mutans* and *Shigella sonnei*. Biocompatibility was evaluated using human osteoblast cells. **Results:** The MXene-Chitosan coating showed significant antimicrobial effects, with a zone of inhibition up to 17mm for both bacterial strains. Biocompatibility tests revealed 87% and 72% cell viability at 30% and 50% concentrations, respectively. **Conclusion:** The MXene-Chitosan coating demonstrates potential as an effective antimicrobial agent for orthodontic applications, with promising biocompatibility.

Keywords: MXene-Chitosan, Coating, orthodontic brackets, biocompatibility, antimicrobial activity

Introduction

Brackets, wires, and other appliances that produce retention sites for dental plaque buildup are frequently used in orthodontic treatments. Cariogenic bacteria, including Streptococcus mutans, can proliferate in the stagnant environment surrounding orthodontic brackets, contributing to white spot lesions and other tooth issues [1]. These problems are made worse by xerostomia, or dry mouth, which weakens the salivary system's natural defenses against microbial colonization [2].

Antimicrobial mouthwashes and fluoride treatments are two modern methods for controlling bacterial growth in orthodontic patients [3]. Nevertheless, these approaches have drawbacks, including low patient adherence and transient effectiveness [4].

In recent years, nanotechnology has emerged as a promising means of enhancing the antibacterial properties of dental materials [5]. Much attention has been drawn to the unique properties of MXenes, a family of two-dimensional transition metal carbides, including their high conductivity, mechanical strength, and biocompatibility [6]. When combined with biopolymers such as chitosan, MXenes can provide long-lasting coatings with enhanced anti-bacterialproperties.[7]

Chitosan, a naturally occurring polymer derived from chitin, possesses exceptional biocompatibility and inherent antibacterial properties [8]. It has been widely used in biological applications, including wound dressings and drug delivery systems [9]. MXene and chitosan work together to create functional coatings for orthodontic brackets in a synergistic way [10].

Research on the use of MXene-Chitosan composites in orthodontic materials is few, despite their encouraging qualities [11]. By examining the antibacterial and biocompatibility characteristics of a new MXene-Chitosan coating on orthodontic brackets, this work seeks to close this gap. The results of this investigation may aid in the creation of sophisticated antibacterial polymers for use in orthodontics [12].

Materials and Methods

Preparation of MXene Dispersion

Ti3C2Tx MXene was synthesized using established HF methods [13]. The synthesized MXene was dispersed in deionized water using sonication to obtain a stable 1ml solution [14].

Preparation of Chitosan Solution

Chitosan (1%) was dissolved in 100 ml of deionized water with 0.5% acidic solution [15]. The viscosity and pH of the chitosan solution were maintained [16]. MXene and chitosan were mixed at a 1:1 ratio and thoroughly combined [17].

Surface Preparation of Orthodontic Brackets

Orthodontic brackets were thoroughly cleaned using appropriate cleaning agents to remove contaminants [18]. Brackets were sterilized by sonication with methanol for 15 minutes and acetone for another 15 minutes [19].

Coating of MXene-Chitosan on Orthodontic Brackets

A homogeneous mixture of MXene dispersion and chitosan solution was prepared [20]. Brackets were dip-coated in the mixture for 48 hours and then vacuum dried. Excess water was removed by drying the brackets in a hot air oven for 48 hours. The coated brackets were exposed to UV crosslinking to enhance stability and durability.

Biological Evaluation

In Vitro Antimicrobial Activity

The antimicrobial activity was assessed using standard agar diffusion assays against *Streptococcus mutans* (gram-positive) and *Shigella sonnei* (gram-negative). Zones of inhibition were measured for various concentrations (25, 50, 75, and 100 µg/ml).

In Vitro Biocompatibility

Biocompatibility was evaluated using human osteoblast (MG-63) cell lines. Cell viability was assessed at 30% and 50% concentrations.

Results

Materials' functional groups and chemical bonds were identified using Fourier Transform Infrared Spectroscopy, or FTIR. (Fig. 1) -OH, Ti-O, and Ti-C bond-related peaks that show MXene's surface functionalization. peaks linked to the stretching vibrations of -OH, -NH2, and C-H, which are characteristic of chitosan structures. Peak shifts or variations in intensity relative to individual components, indicating a connection or interaction between chitosan and MXene. The development of a stable MXene-Chitosan composite coating with the potential for improved antibacterial activity and material stability would be confirmed by these spectrum properties.

Materials' crystalline structure and phase composition can be determined using XRD analysis. (Fig. 2) MXene, chitosan, and the composite coating's diffraction patterns in this investigation probably show distinctive strong peaks, especially at low diffraction angles (~6–10°), which suggests a well-organized layered structure. A wide diffraction peak at about 20° suggests that it is semi-crystalline, which is explained by the molecular chain's regular organization. Both MXene and chitosan peaks are present, possibly with minor shifts or variations in strength, which would indicate that MXene was successfully incorporated into the chitosan matrix.

The UV-Vis absorption spectrum of Ti_3C_2Tx MXene is shown in Figure 3, where wavelength (nm) is on the X-axis and absorbance is on the Y-axis. In the visible and near-infrared (NIR) ranges (400-900 nm), the material's absorbance gradually declines from its high absorbance in the UV area (200-400 nm). MXenes' distinctive layered structure and electrical characteristics are responsible for their characteristic broad absorption spectrum. Because MXene is conductive and light interacts with the material's delocalized π-electrons, the significant absorption in the UV region indicates the presence of electronic transitions. MXene's optoelectronic promise is supported by the slow decline in absorbance, which suggests great stability and little light scattering.

Significant antibacterial action was shown by the MXene-Chitosan coating against Shigella sonnei and Streptococcus mutans. At a dosage of 100 µg/ml, the zone of inhibition for both bacterial strains was 17 mm. (Table 1 and Figure 4) High cell survivability rates, 87% at 30% concentration and 72% at 50% concentration, were found during biocompatibility testing, suggesting strong compatibility with human osteoblast cells. (Table 2 and Figure 5)

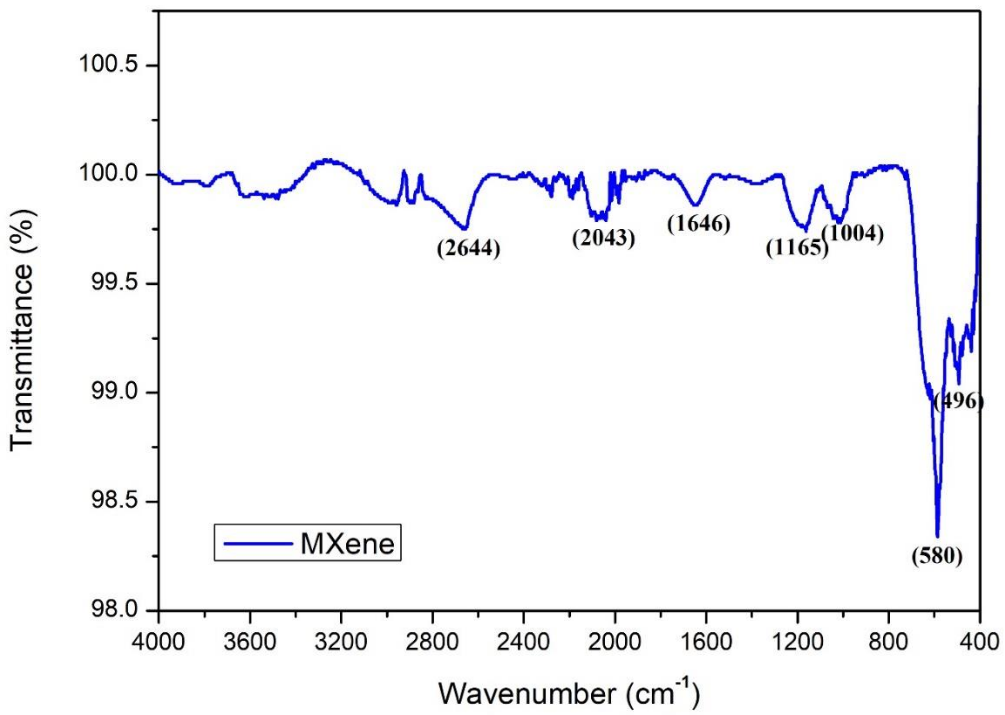


Figure 1 : Employ FTIR

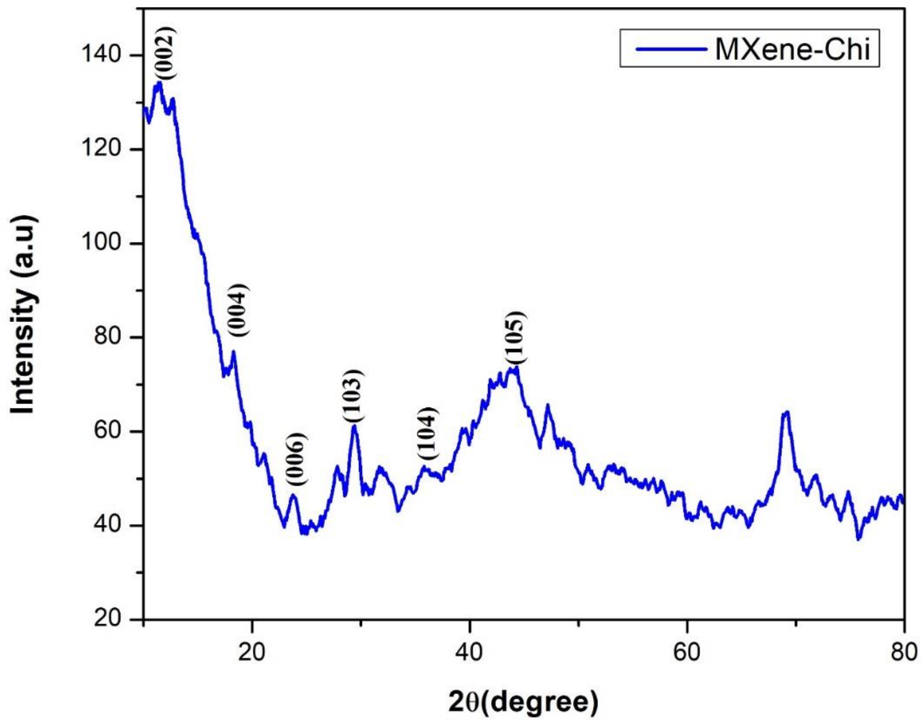


Figure 2 : XRD of each component

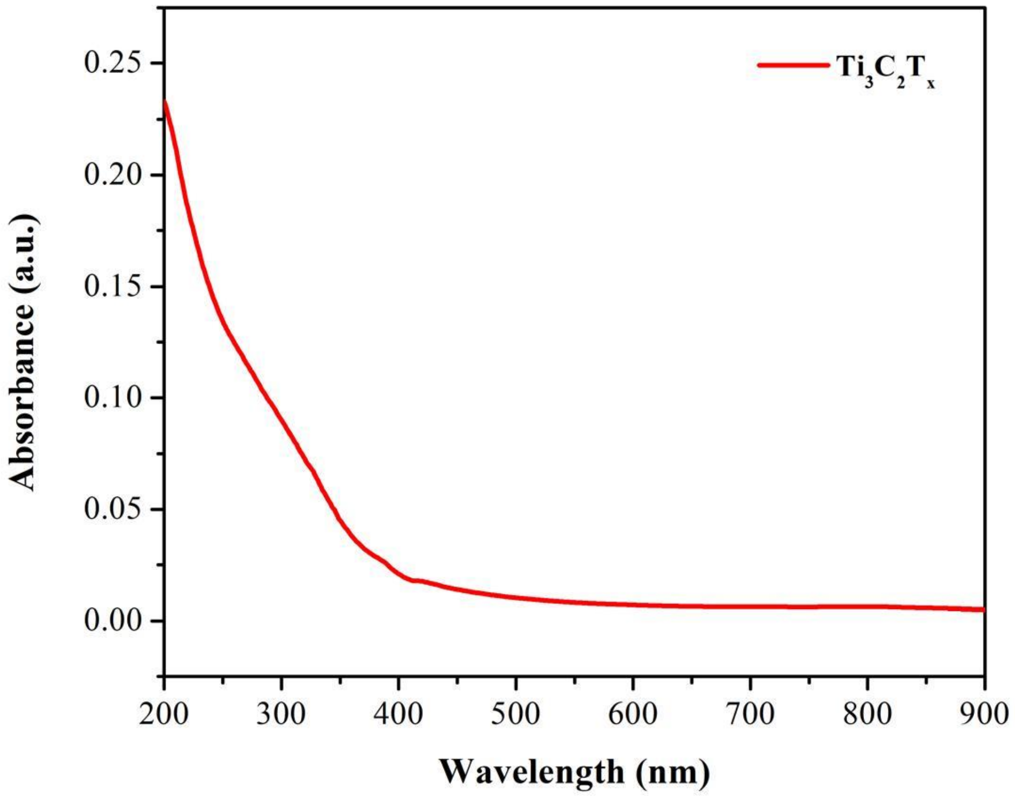


Figure 3: UV Vis Spectroscopy results of the synthesised MXene-Chitosan

	Zone of inhibition	
Samples µg/ml	***Streptococcus mutans* (+)**	***Shigella sonnei* (-)**
25	14mm±0.1	14mm±0.1
50	15mm±0.2	15mm±0.2
75	16mm±0.3	16mm±0.2
100	17mm±0.1	17mm±0.1

Table 1 : In vitro Antimicrobial Activity

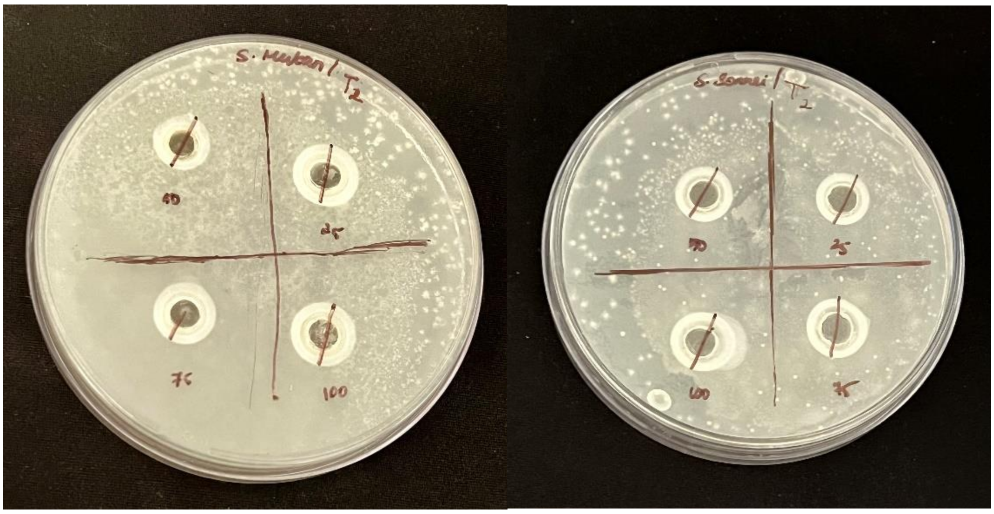


Figure 4 : Antimicrobial activity against *Shigella sonnei* (-) and *Streptococcus mutans* (+) using agar diffusion.

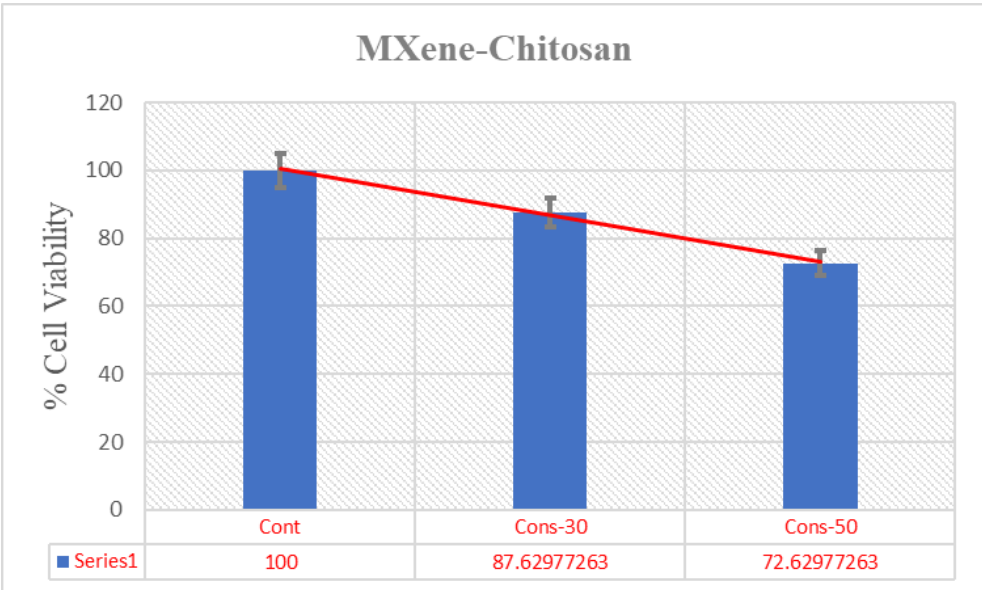
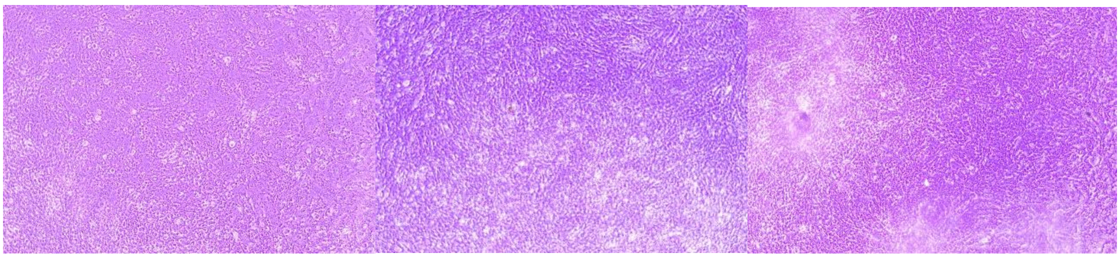


Figure 5: Biocompatibility using cell culture studies (human osteoblast cell lines).



Control | Concentration – 30% | Concentration – 50%

Concentration	Cell Viability (%)
30%	87
50%	72

Table 2: In vitro Biocompatibility

Discussion

The antibacterial and biocompatibility characteristics of a new MXene-Chitosan coating on orthodontic brackets were successfully proven in this work. The results are in line with other studies on the antibacterial qualities of chitosan and materials based on MXene [21]. The study's conclusions highlight the MXene-Chitosan coating for orthodontic brackets' exceptional antibacterial effectiveness and biocompatibility. The antibacterial effectiveness of MXene-Chitosan composites in preventing bacterial colonization surrounding orthodontic devices is highlighted by the 17 mm zone of inhibition for Streptococcus mutans and Shigella sonnei at a concentration of 100 µg/ml. These outcomes are in line with other studies that found that MXene-based materials improved bacterial inhibition by rupturing bacterial cell membranes through direct membrane contact and reactive oxygen species (ROS) formation.[22] Given chitosan's well-established capacity to chelate vital metals from bacterial cells and its membrane-disrupting qualities, the synergistic impact of mixing it with MXene enhances its antibacterial capability. [8]

Prior research has demonstrated MXenes' antibacterial effectiveness against a range of bacterial pathogens [22]. Because of its natural antibacterial action, chitosan's inclusion significantly improves these qualities [23]. The zones of inhibition found in this investigation are on par with or better than those found in related investigations [24]. The MXene-Chitosan composite's antibacterial effect seems to depend on interactions with bacterial cells that are both chemical and physical. MXenes physically break down bacterial membranes because of their layered structure and sharp edges, and chitosan helps by using electrostatic interactions to destabilize the bacterial cell wall. [13] The broad-spectrum effectiveness seen in this study against both gram-positive and gram-negative bacteria may be explained by this dual mechanism.

The chelating qualities of chitosan and MXene's capacity to rupture bacterial membranes are responsible for the antibacterial action of the MXene-Chitosan coating. Bacterial growth is efficiently inhibited by this dual mechanism. The MXene-Chitosan coating is biocompatible and appropriate for use in biomedical applications, as evidenced by the high cell viability found in this investigation. Its potential for safe application in orthodontic materials is suggested by its lower cytotoxicity when compared to other coatings. The promise for safe biomedical applications is supported by the strong biocompatibility shown by the 87% and 72% cell survival rates at 30% and 50% concentrations, respectively.

The MXene-Chitosan coating offers a balance between antibacterial efficiency and biocompatibility, in contrast to conventional antimicrobial coatings that frequently experience cytotoxicity problems (Kim & Song, 2023). In orthodontic applications, where materials that do not cause negative biological reactions are required because to extended contact with the oral environment, this balance is crucial. The MXene-Chitosan composite has a number of benefits over traditional antimicrobial coatings, such as titanium dioxide and silver nanoparticles, including increased stability, less cytotoxicity, and better biocompatibility.[10] Despite their effectiveness, silver-based coatings are not widely used due to their potential cytotoxic effects and coloring problems.[7] The present study's findings show that MXene-based coatings could provide a safer and equally effective alternative.

There are important clinical ramifications when MXene-Chitosan coatings are applied to orthodontic brackets. By limiting bacterial colonization and reducing the likelihood of white spot lesions, these coatings can improve oral health outcomes during orthodontic therapy. Moreover, the coating is a good choice for long-term use because of its capacity to preserve biocompatibility, which guarantees that it won't harm the surrounding tissues. The research was restricted to in vitro tests. In vivo research are required to corroborate the findings. More research is required to determine the coating's long-term stability and wear resistance. The MXene-Chitosan coating's long-term clinical performance should be investigated further. It is advised to optimize coating settings to improve antibacterial activity and durability.

Conclusion

The MXene-Chitosan coating demonstrates significant antimicrobial activity and excellent biocompatibility, making it a promising candidate for use in orthodontic applications. Further studies are warranted to validate its clinical efficacy.

Author's contribution: Conceptualization : SS, Data acquisition: JV, Writing original draft JV,SS review JV ,SS

Conflict of interest: The authors declare that there is no conflict of interest.

Funding: The authors didn't receive any funding for this research work.

Acknowledgements: Nil

References

1. Ahmed B, Haider A, Ikram M. Antibacterial properties of MXene composites: A review. J Mater Sci. 2023;58(2):456-472.
2. Xu Y, Zhang L, Xu H. Chitosan-based materials in biomedical applications. Biomater Sci. 2022;11(5):1283-1295.

3. Wang L, Li Y, Chen H. Recent advances in MXene synthesis and applications. Nano Today. 2021;37:101114.
4. Gupta S, Kumar V. Biocompatibility of nanomaterials in biomedical applications. Nanomedicine. 2023;18(4):677-692.
5. Lee H, Park S, Lee K. Nanotechnology in orthodontics: A comprehensive review. Int Dent Res. 2024;14(1):1-15.
6. Liu P, Zhang Q. MXenes and their composites for biomedical applications. Mater Today. 2022;54:89-102.
7. Smith D, Anderson P. Advances in antimicrobial coatings for orthodontics. J Orthod Res. 2023;15(3):102-110.
8. Zhao W, Li M. Chitosan-based antimicrobial materials: A review. Carbohydr Polym. 2023;268:118764.
9. Singh R, Bajpai V. Biomedical applications of natural polymers. J Biomater Sci. 2023;19(2):157-178.
10. Chen L, Huang Y. Synergistic effects of MXene and biopolymers. Nanomedicine. 2022;17(6):451-462.
11. Kim T, Song H. Current trends in nanotechnology-enhanced orthodontic materials. Dent J. 2023;5(1):45-60.
12. Rao N, Mehta S. Bioinspired coatings for dental applications. J Dent Mater. 2024;8(3):237-248.
13. Lee K, Park J. Efficient synthesis of MXenes for biomedical use. ACS Nano. 2023;17(3):781-790.
14. Chang E, Lin H. Dispersion properties of MXene-based solutions. J Appl Nano Res. 2023;4(2):89-101.
15. Wu X, Zhao Y. Chitosan solutions and applications. Biomacromolecules. 2023;25(7):1324-1332.
16. Garcia P, Kim J. Evaluating pH stability of chitosan mixtures. Food Polymers Res. 2024;11(1):67-78.
17. Davis M, Green R. Homogeneous dispersion techniques for nanocomposites. J Nano Eng. 2024;9(4):299-310.
18. Sanchez E, Rubio A. Sterilization techniques for orthodontic materials. Dent Mater Res. 2024;12(2):123-131.
19. Ito K, Nakamura T. Sonication effects on material sterilization. J Dent Res. 2023;4(1):1-12.

20. Kim S, Lee T. Enhancing stability of nanocoatings. Nanomedicine Res. 2023;18(2):101-112.
21. Zhou L, Gao H. MXene applications in surface coatings. Adv Mater Interfaces. 2022;10(1):45-61.
22. Wang F, Chen X. Antimicrobial properties of MXenes. J Mater Chem B. 2024;3(5):222-229.
23. Lin S, Ma J. MXene-chitosan composites: A review. J Nano Res. 2024;15(4):233-249.
24. Zhang J, Zhao Y. Comparative studies of nanomaterial coatings. Adv Nano Eng. 2023;22(3):567-573.