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Development of Polypropylene/MoO_3 Nanocomposite Fibers to Evaluate Antimicrobial, Antiviral, and UV-Protective Performance

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Abstract

The growing demand for polymeric materials with functional properties drives the development of nanocomposites capable of simultaneously meeting hygiene, health, and safety requirements. In this context, the present study investigates the incorporation of molybdenum trioxide (MoO_3) nanoparticles into polypropylene (PP) fibers produced by melt spinning, focusing on the evaluation of their antimicrobial, antiviral, and UV protection properties. The produced samples demonstrated significant activity against pathogenic microorganisms such as *Staphylococcus aureus* and *Escherichia coli*, achieving over 99% bacterial reduction with low nanoparticle content. However, the results obtained for UV protection and coronavirus activity were not satisfactory under the tested conditions. Further research is required in these areas to deepen the understanding and enhance performance.

Keywords

Molybdenum Trioxide, Polypropylene Fibers, Antibacterial, Antiviral, UV Protection, Functional Textiles

1. Introduction

The integration of advanced functionalities into polymeric materials has become increasingly important to address the growing demands for safety, hygiene, and performance in industrial, medical, and consumer applications. Among these materials, polypropylene (PP) nanocomposite fibers stand out due to their versatility, low cost, light weight, and recyclability, combined with the

possibility of tailoring their performance through the incorporation of functional nanofillers [1] [2].

Key challenges for polymeric systems employed in critical environments or human-contact applications include the need for antimicrobial and antiviral activity, as well as protection against ultraviolet (UV) radiation. Microbial growth on polymer surfaces not only compromises product integrity but also poses risks to human health, while biofilm formation is particularly problematic in medical, packaging, and technical textile sectors [3] [4]. Moreover, the inherently poor UV resistance of PP represents a major limitation for its outdoor and protective clothing applications [5].

To overcome these limitations, a wide range of nanoparticles has been investigated, particularly metal oxides such as ZnO, TiO_2, CuO, and Ag, which have demonstrated antimicrobial, UV-shielding, and in some cases antiviral properties [6]-[13]. Despite these promising results, concerns regarding biocompatibility, environmental safety, and cost have restricted their broader implementation.

Molybdenum trioxide (MoO_3) has recently gained attention as a multifunctional alternative. It exhibits broad-spectrum antimicrobial activity, still underexplored antiviral potential, low toxicity, high thermal stability, and strong compatibility with polymer matrices [14]-[19]. Its antimicrobial action is primarily attributed to the slow release of acidic species (H^+ and MoO_4^{2-}), which destabilize bacterial membranes and induce cell death even in the absence of UV irradiation [15] [16]. In addition, although not traditionally considered a UV-blocking material like TiO_2 and ZnO, MoO_3 displays interesting photocatalytic interactions with UV radiation. Its semiconducting band gap enables photon absorption, and the orthorhombic phase in particular exhibits effective UV absorption [20] [21].

Despite these promising characteristics, the use of MoO_3 nanoparticles in PP fibers remains scarcely explored, especially with a combined focus on antimicrobial, virucidal, and UV-protective functionalities. This knowledge gap highlights the need for systematic studies that address not only functionality but also processing feasibility and sustainability.

Therefore, the present work investigates the incorporation of MoO_3 nanoparticles into PP fibers produced by melt spinning, aiming to evaluate their antimicrobial, antiviral, and UV-protection properties. The study provides insights into the multifunctional potential of MoO_3 as an additive for advanced polymer nanocomposites and technical textiles, continuing ongoing research efforts (data under publication).

2. Experimental

2.1. Materials

The isotactic homopolymer PP, grade H 201, was supplied in pellet form by Braskem S.A. According to the product datasheet, it is a fiber-grade polypropylene

(PP) resin with a high melt flow index (MFI) of 20 g·10 min^{-1}, good melt stability, a normal molecular weight distribution, and a density of 0.905 g·cm^{-3}, making it suitable for fiber extrusion or injection molding.

Molybdenum trioxide (VI) powder, with 99.5% purity, particle size of 100 nm, and CAS number 1313-27-5, was purchased from Sigma-Aldrich Co. and used as the filler in PP fibers.

SPAN 80 (sorbitan monooleate), a surfactant with molecular formula $C_{24}H_{44}O_6$, molecular weight 428.62 g·mol^{-1}, and CAS number 1338-43-8, was obtained from Inlab Confiança and employed as a compatibilizing agent to improve the dispersion of MoO_3 in the PP masterbatch.

Delion FA-1055 finishing oil, acquired from Takemoto Oil & Fat CO., was used as a lubricating auxiliary during the melt spinning of the filaments. According to its datasheet, it is a mineral oil containing synthetic lubricants and a combination of nonionic and anionic surfactants.

Fluowet UD, a wetting agent purchased from CHT, was used in this study for the antimicrobial evaluation to render the PP hydrophilic. The wetting detergent Trewet AC, obtained from Tremembé Indústrias Químicas, along with glacial acetic acid and sodium hydroxide pearls from Química Moderna, were employed in the purge process of the fabrics produced from the filaments.

2.2. Preparation of the PP/MoO_3 Masterbatch

To achieve better nanoparticle dispersion within the fibers, a masterbatch containing 5 wt% MoO_3 was produced. Molybdenum trioxide nanoparticles (15 g) were physically mixed with 285 g of virgin PP pellets, along with 2 mL of SPAN 80 (sorbitan monooleate), and fed into the hopper of a co-rotating intermeshing twin-screw extruder (L/D = 30), model Teach Line ZK25T from Dr. Collin GmbH, Germany with eight heating zones. The extruder was coupled to a pelletizer, yielding 300 g of masterbatch. The temperature profile during extrusion was as follows: 135˚C (zone 1), 155˚C (zone 2), 165˚C (zone 3), 175˚C (zone 4), 185˚C (zone 5), 200˚C (zone 6), 205˚C (zone 7), and 215˚C (zone 8). The screw rotation speed was set at 100 rpm, the dosing pump at 20 rpm, and the melt pressure at 42 bar. The residence time in the extruder was approximately 5 minutes.

2.3. Preparation of PP/MoO_3 Nanocomposite Fibers

The nanocomposite fibers were produced via melt spinning using a co-rotating, intermeshing twin-screw extruder (L/D = 30, Teach Line ZK25T, Dr. Collin GmbH, Germany). The polymer and nanoparticle concentrations, as well as the fiber codes, are summarized in Table 1. A control run without additives was performed under the same processing conditions; in this case, SPAN 80 was not used because sorbitan monooleate undergoes thermal degradation at temperatures lower than those used for processing the nanocomposite fibers, as previously reported. The temperature profile during fiber extrusion and other processing parameters were also described in previous work.

Table 1. Identification of the fibers samples produced.

Sample	Polymeric matrix	Load	Load content* (wt%)
S0	PP	-	0
S1	PP	MoO_3	0.1
S2	PP	MoO_3	0.2
S3	PP	MoO_3	0.5

*Values determined by ICP-OES.

3. Fabric Production and Alkaline Purging Process

After filament processing, knitted fabrics were produced using a circular knitting machine for subsequent evaluation of UV protection. The machine used was a Lab Knitter 294E (Mesdan S.P.A., Italy).

The fabrics were then subjected to an alkaline purging process to remove the finishing oil applied during melt spinning, ensuring that it would not interfere with characterization results. The purging treatment was carried out in an ATHT-1 equipment (Kimak, Brazil). Each material was immersed in separate containers containing an aqueous solution of 2.0 $mL \cdot L^{-1}$ of the wetting detergent Trewet AC and 15 $mL \cdot L^{-1}$ of sodium hydroxide at 36˚Bé. The bath-to-material weight ratio was 10:1, and the fabrics were mechanically agitated at 90˚C for 60 minutes.

Subsequently, the bath was cooled to 40˚C, discarded, and the samples were rinsed under running tap water. The fabrics were then subjected to the same equipment in a fresh bath containing 1 $mL \cdot L^{-1}$ of acetic acid to neutralize the material's pH, for 10 minutes at 40˚C. Finally, the fabrics were removed, thoroughly rinsed with cold water to eliminate any residual chemicals, and air-dried at room temperature.

3.1. Characterizations

The materials used for characterization were stored in a cabinet and conditioned prior to each analysis according to the environmental conditions specified in the respective methodologies.

Filament samples were evaluated for antimicrobial activity following the AATCC TM 100-2019 standard [22]. The tests employed *Staphylococcus aureus* (American Type Culture Collection, ATCC No. 6538) as the Gram-positive microorganism and *Escherichia coli* (ATCC No. 25922) as the Gram-negative microorganism. Specimens weighing approximately 1 g were used directly without prior sterilization. The bacterial inoculum concentration ranged from 1 - 3 × 10^5 $CFU \cdot mL^{-1}$.

Samples were placed in Petri dishes, inoculated with the bacterial suspension, and incubated at 37 ± 2˚C for 24 hours for each analysis. After the incubation period, colony counts were determined using an automatic colony counter. Antibacterial activity was expressed as the percentage of bacterial reduction, calculated using Equation (1):

$$\%R = \frac{100(B - A)}{B} \quad (1)$$

Where %R is the percentage of bacterial reduction, A is the number of bacteria recovered from the sample containing MoO_3 nanoparticles, and B is the number of bacteria recovered from the control sample.

3.2. UV Protection

The UV protection of the knitted fabrics produced from filaments containing molybdenum trioxide was evaluated in comparison with a control fabric without the filler. For a total of eight measurements, four specimens were tested, with two measurements per specimen. A Perkin Elmer UV-VIS spectrophotometer (Lambda 800, S/N 101N4021301) equipped with a PELA-1000 accessory (SC-0226) and calibrated by SENAI CETIQT - CSM/Colorimetry Laboratory (Certificate No. 2078/24, dated 17/07/2024) was used. Data acquisition was performed using the WinLab software, version 5.1.5. Environmental conditions were controlled at 20.0 ± 5.0˚C and relative humidity of 45% - 70%, monitored with a Hanna Instruments thermo-hygrometer (HI9564, S/N G0030749, SC-0437; Calibration Certificate LT-417 284, 08/01/2024). The methodology was based on the AS 4399:2020 standard [23].

3.3. Antiviral Activity

The antiviral activity of the nanocomposite filaments and the control samples was evaluated using an adaptation of ISO 18184:2025 [24], employing Vero cells and virus quantification via the Tissue Culture Infectious Dose 50% ($TCID_{50}$) method. The textile samples were analyzed in three steps: cytotoxicity assessment, antiviral screening against the Measles virus (as a preliminary respiratory virus model in BSL-2), and antiviral testing against SARS-CoV-2 in BSL-3.

Briefly, after cytotoxicity was confirmed, 20 mm samples of control and formulated textiles were exposed to virus suspensions for 24 hours at room temperature (contact: yarn plus virus). Subsequently, the samples were washed to recover the virus, and viral titers were quantified using the $TCID_{50}$ method on Vero CCL-81 cells. Antiviral performance was classified according to the reduction in viral titer: differences of 2.0 - 3.0 log $TCID_{50}$/mL were considered a good effect (antiviral efficacy > 99%), while reductions higher than 3.0 log $TCID_{50}$/mL were considered excellent (antiviral efficacy > 99.9%).

4. Results and Discussion

4.1. Antimicrobial Effect

The antibacterial activity of the PP/MoO_3 nanocomposite fibers was investigated, and the results are summarized in **Table 2**. Against *S. aureus*, the sample containing only 0.1 wt% MoO_3 exhibited the highest reduction in colony-forming units (CFU), achieving an 83% reduction compared to the pure PP sample. However, samples with higher nanoparticle concentrations did not show a significant reduction for this strain. In contrast, all samples containing MoO_3 were effective against the Gram-negative strain *E. coli*, with bacterial reduction percentages ex-

ceeding 90%.

Table 2. Antimicrobial efficiency of the samples using AATCC TM 100:2019.

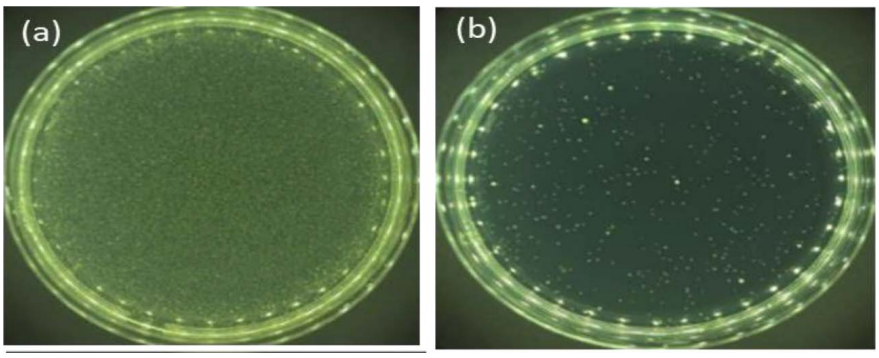
Samples	%R without wetting agent to *S. aureus* ATCC 6538	%R without wetting agent to *E. coli* ATCC 25922	%R with wetting agent to *S. aureus* ATCC 6538
S0	0	0	0
S1	83.0	99.0	98.0
S2	35.0	94.0	99.8
S3	29.0	99.0	99.9

Erem *et al.* [25] and Suntamit *et al.* [26] reported in their respective studies that the inherent hydrophobic nature of polypropylene fibers impaired the expected antibacterial activity when ZnO nanoparticles were incorporated into this polymer. According to these authors, the antimicrobial efficiency of the fibers increased after improving their water absorption capacity.

To achieve better results against the Gram-positive strain *S. aureus*, an additional round of testing was performed by adding a wetting agent to the AATCC 100:2019 methodology [22]. During the bacterial inoculation step, 10 $g{\cdot}L^{-1}$ of the wetting agent Fluowet UD was used. The role of this product is to "transport" the bacterial inoculum into the fibers so that the metal nanoparticles can exert their effect. A preliminary test using only the wetting agent with the control sample confirmed that Fluowet UD does not possess activity against the strains tested in this study.

With the addition of the wetting agent, the bacterial reduction percentages against *S. aureus* increased from 83% to 98% in sample S1, and from 35% and 29% to 99.9% in samples S2 and S3, respectively (**Table 2**). The bactericidal mechanism of MoO_3 nanoplatelets is attributed in the literature to the release of acidic species such as H^+ and MoO_4^{2-} or hydronium ions (H_3O^+), which affect enzymatic activity, protein stability, and nucleic acid structure of the bacterial cell membrane, ultimately inactivating the microorganisms [27] [28].

Figures 1 and **2** illustrate the CFU counts present in the Petri dishes for the control sample and for samples S1, S2, and S3 against *S. aureus* and *E. coli*, respectively, without the wetting agent.



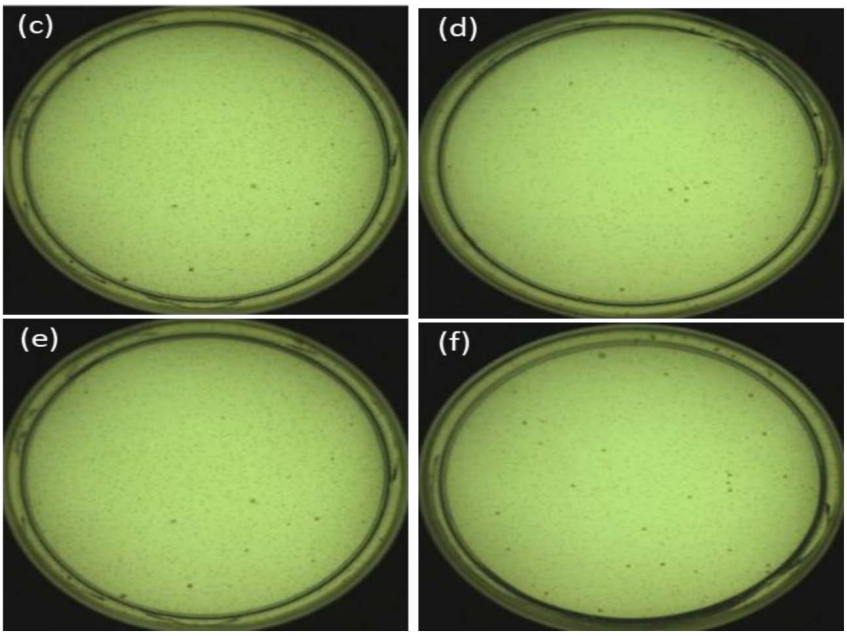


Figure 1. (a), (c) and (e) No. of bacteria recovered from the sample S0 and no. of bacteria recovered from the samples: (b) S1 with %R = 83%, (d) S2 with %R = 35% and (f) S3 with %R = 29% both after 24 h of incubation time against *Staphyloccocus aureus* without wetting agent.

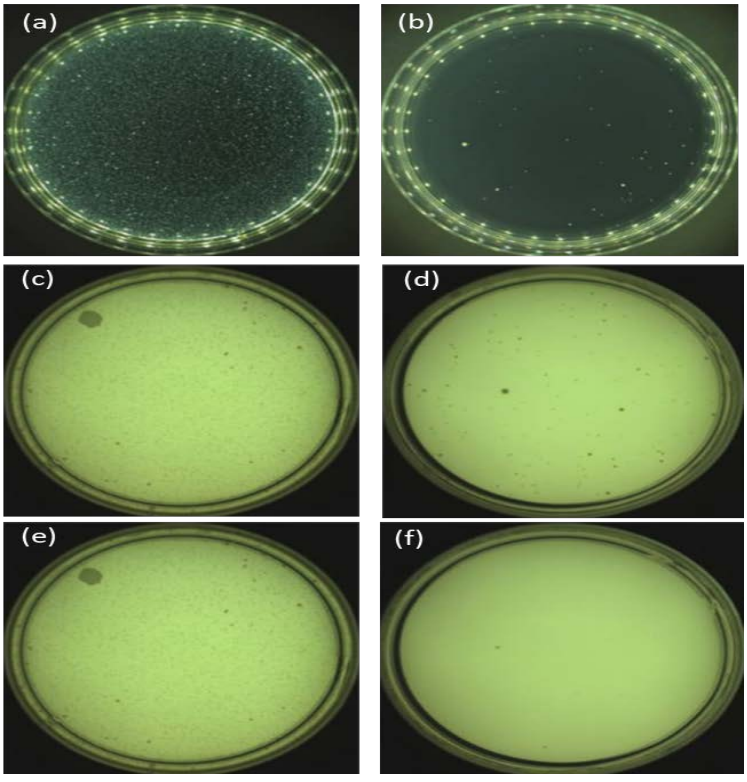


Figure 2. (a), (c) and (e) No. of bacteria recovered from the sample S0 and no. of bacteria recovered from the samples: (b) S1 with %R = 99.0%, (d) S2 with %R = 94.0% and (f) S3 with %R = 99.0% both after 24 h of incubation time against *Escherichia coli* without wetting agent.

Figure 3 shows the bacterial counts in the Petri dishes for the control sample and samples S1, S2, and S3 against the *S. aureus* strain after the application of the wetting agent.

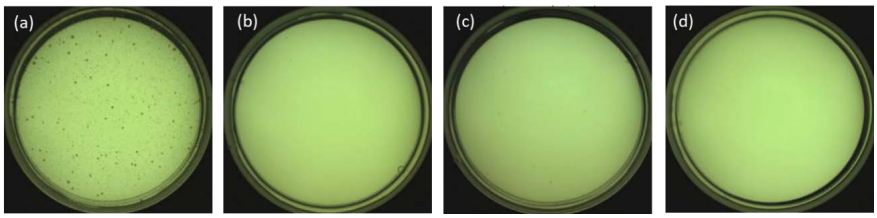


Figure 3. (a) No. of bacteria recovered from the sample S0 and no. of bacteria recovered from the samples: (b) S1 with %R = 98.0%, (c) S2 with %R = 99.8% and (d) S3 with %R = 99.9% both after 24 h of incubation time against *Staphyloccocus aureus* with wetting agent.

4.2. UV Protection

In the evaluation of the ultraviolet protection factor (UPF) according to the AS 4399:2020 standard [23], the spectral transmittance of UV radiation through the fabric is measured, *i.e.*, the amount of radiation that passes through the sample. Higher transmittance values correspond to lower protection provided by the substrate, and vice versa. According to the standard, the UPF calculation is not based on the simple average of transmittances but is weighted by the solar spectrum and the erythemal response of the skin. The formula and classification system for UPF are provided by the standard.

A UPF value of 15 corresponds to a "minimal" protection rating, 30 is considered "good," and 50 or higher is classified as "excellent." Values below 15 are considered by the standard as materials that do not provide UV protection.

The results for the average UPF values obtained from the measurements of the pure fabric and fabrics containing molybdenum trioxide, as well as the transmittance values (T%) for the UVA (315 - 400 nm) and UVB (290 - 315 nm) ranges and the corresponding classifications based on AS 4399:2020, are presented in Table 3.

Table 3. The UVA and UVB transmittance values, the corresponding UV protection factor (UPF), and the classification of the knitted fabric samples, both pure and containing MoO_3.

Samples	T% (UVA)	T% (UVB)	Values of UPF	Classification AS 4399:2020
S0	32.6108	26.1130	4	<15
S1	30.8673	21.1232	4	<15
S2	51.2918	47.8664	2	<15
S3	34.2068	26.1654	4	<15

Note: The standard deviation of the four specimens tested in terms of UPF was equal to 0.

As observed, none of the samples exhibited satisfactory UV protection. Sample S1, containing only 0.1 wt% MoO_3, showed lower transmittance values (UVA and UVB) compared to the other MoO_3-containing samples and the pure fabric. This

result may be related to the better dispersion of nanoparticles within the fibers in this sample.

Although no studies correlating the amount of molybdenum trioxide with UPF values were found, research with analogous UV blockers, such as TiO_2 and carbon nanotubes, indicates that higher filler content generally leads to increased UV protection [29] [30]. Therefore, a broader investigation using higher MoO_3 concentrations within practical and safety limits is necessary to evaluate potential improvements in UV-blocking performance.

Unlike well-established UV-protective materials, research on MoO_3 has focused more on photocatalytic applications rather than direct UV protection [31]-[37]. The primary UV-protection mechanism of MoO_3 relies on photocatalytic degradation rather than physical blocking [21], which may limit its applicability in conventional solar protection or UV-blocking

4.3. Application Antiviral

As previously mentioned, the yarn samples were first evaluated for cytotoxic effects on Vero cells and for potential interference with cellular susceptibility to viral infection using the Measles virus. All samples were deemed suitable to proceed to the antiviral assay against SARS-CoV-2, as they did not exhibit a difference greater than 0.5 log $TCID_{50}$ compared to the control sample.

However, no antiviral activity against the virus responsible for COVID-19 was detected in any of the samples, as shown in **Table 4**. According to ISO 18184:2025 [24], viral infection inhibition is considered absent if the reduction in log $TCID_{50}$ for the samples under analysis is less than or equal to 1 compared to the control.

Table 4. Antiviral Activity Results of MoO_3-Containing Samples versus the Control Sample.

Samples	Log Title $TCID_{50}$/mL	Difference between Sample Control and treated sample Log $TCID_{50}$/mL	reduction antiviral efficiency Log $TCID_{50}$
S0	5.35	-	-
S1	5.33	0.02	No antiviral activity was detected
S2	5.81	−0.46	No antiviral activity was detected
S3	6	−0.65	No antiviral activity was detected

As previously discussed in the evaluation of antimicrobial effects, the antiviral mechanisms reported for MoO_3 focus on surface chemistry and catalytic activity. Although direct, peer-reviewed data on efficacy against specific human viruses are scarce and mostly indirect, reviews and some experimental studies report catalytic oxidation, the generation of reactive oxygen species (ROS)/peroxides, and local acidity from proton release as the main modes of action of molybdenum oxide that can damage microbes or viral components [38]-[40].

According to Lee *et al.* [41], MoO_3 nanoplatelets act as enzyme-mimetic catalysts, producing ROS that can inactivate pathogens via oxidation of proteins, lipids, or nucleic acids. Shafaei *et al.* [42] reported that high-surface-area MoO_3 particles incorporated into polymers release protons at the surface, creating localized acidity that impairs microbial viability and can destabilize viral envelopes or proteins in close contact with the material surface.

Given this, it is suggested that the hydrophobic nature of PP negatively influenced the release of reactive species and protons, preventing effective interaction with the coronavirus. Studies such as Achadu *et al.* (2021) [40] highlight the value of molybdenum for diagnostic applications and biosensing, rather than for direct antiviral treatment.

Recent studies have indicated that molybdenum-based materials (e.g., MoO_3 and molybdate compounds) exhibit antimicrobial and antiviral activity mediated by multiple mechanisms, including the release of soluble ionic species (molybdate), the generation of reactive oxygen species (ROS), and direct interaction with viral surface components that may lead to protein denaturation and damage to genetic material (RNA/DNA) [42] [43]. Antiviral efficiency has also been associated with the physicochemical properties of nanomaterials, such as high surface area, oxygen vacancies, and lattice defects that enhance surface redox reactions and increase reactivity [44].

5. Conclusions

The results of this study demonstrate that PP/MoO_3 nanocomposites are a promising alternative for the development of functional polymeric materials, particularly in applications requiring antimicrobial activity. For broader applications involving UV protection and antiviral performance, further research is still necessary, including systematic variation of nanoparticle loading, exploration of synergistic effects with other metal oxides, and implementation of strategies to mitigate the intrinsic hydrophobicity of PP.

Overall, PP/MoO_3-based fibers and textiles exhibit strong potential to enhance user protection by combining multifunctionality, industrial feasibility, and sustainability. These findings provide not only a foundation for the design of advanced polymeric systems with tailored performance but also valuable insights to guide future developments toward safer and more effective antimicrobial and antiviral materials.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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