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# Improvement Mechanism of Dielectric and Mechanical Properties of Organic-Polymer-Based Functional Nanocomposites via Nanofiller Interface Modification

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## ABSTRACT

Organic-polymer-based functional nanocomposites have outstanding application prospects in flexible electronic devices, energy storage dielectrics, microwave absorption materials and intelligent sensors due to their merits of light weight, facile processing, adjustable flexibility and excellent functional adaptability. Nevertheless, nanofillers suffer from large specific surface area and high surface energy, which inevitably cause severe agglomeration inside polymer matrices. Meanwhile, poor interfacial compatibility and abundant interfacial defects between inorganic nanofillers and organic polymer matrices severely restrict the synchronous improvement of mechanical stability and dielectric performance of composite materials. In this work, thermoplastic polyurethane (TPU) was selected as the organic polymer matrix, and montmorillonite (MMT) nanosheets served as inorganic functional...

Full abstract continues on the metadata continuation sheet.

Index Terms: organic polymer • nanocomposite • interface modification • dielectric property • mechanical property • filler dispersion

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## CONFLICTS

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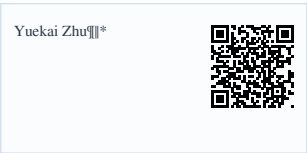
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FULL ABSTRACT

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## RESEARCH ARTICLE

# Improvement Mechanism of Dielectric and Mechanical Properties of Organic-Polymer-Based Functional Nanocomposites via Nanofiller Interface Modification

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## Abstract

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**Keywords:** *organic polymer, nanocomposite, interface modification, dielectric property, mechanical property, filler dispersion*

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## 1 Introduction

### 1.1 Research Progress of Organic-Polymer-Based Functional Nanocomposites

Functional nanocomposites refer to novel composite functional materials fabricated by uniformly dispersing nano-scale inorganic functional fillers into organic polymer matrices, which integrate the superiorities of organic polymers (excellent flexibility, simple molding process and outstanding chemical stability) and inorganic nanofillers (high dielectric constant, high mechanical strength, high thermal conductivity and sensitive electromagnetic response) [1]. Compared with traditional inorganic ceramic functional materials, organic-polymer-based nanocomposites possess irreplaceable advantages including flexibility, light weight, low cost and scalable production. Currently, they have become core substrate

materials for cutting-edge electronic components such as flexible film capacitors, wearable electronic sensors, electromagnetic interference shielding films and flexible piezoelectric devices [2].

Common organic polymer matrices are divided into thermoplastic and thermosetting categories. Thermoplastic polyurethane (TPU) contains hard urethane segments and soft polyether segments in molecular chains, presenting adjustable mechanical elasticity, excellent aging resistance and good filler compatibility. Hence, TPU is one of the most widely applied matrix materials in the field of flexible functional composites [3]. Montmorillonite (MMT) is a typical two-dimensional layered silicate nanofiller with natural lamellar barrier effect and interfacial polarization effect. A small amount of MMT doping can simultaneously enhance the mechanical and dielectric properties of polymer matrices. Besides, MMT has low raw material cost and excellent storage stability, which is suitable for continuous industrial production [4].

Current global researches on polymer-based nanocomposites mainly focus on three directions: filler type selection, matrix formula optimization and preparation process improvement. Existing studies have verified that the dispersion uniformity of nanofillers and interfacial bonding state between two phases directly determine the final comprehensive service performance of composites [5]. Unmodified inorganic nanofillers contain abundant hydrophilic hydroxyl groups on the surface, leading to poor thermodynamic compatibility with hydrophobic organic polymer matrices. Nanoparticles are prone to secondary agglomeration, forming stress concentration points and conductive defect channels inside composites. These defects further result in decreased mechanical strength and sharply increased dielectric loss, failing to meet the long-term stable service requirements of high-end electronic devices [6].

## 1.2 Core Technical Bottlenecks of Current Material systems

Combined with global published research achievements on polymer-based nanocomposites in recent years, three common technical bottlenecks still restrict the large-scale application of such materials:

(1) Filler dispersion bottleneck: Nanofillers have tiny particle size and ultra-high surface energy. Conventional physical preparation methods including melt blending and solution blending cannot completely eliminate particle agglomeration. The size of agglomerates can reach micron level under high filler loading, which directly destroys the continuous phase structure of polymer matrices [7];

(2) Interfacial compatibility bottleneck: Inorganic fillers and organic polymers are heterogeneous materials with obvious molecular chain debonding and cavity defects at the interface. The interface is prone to crack preferentially under external force, reducing the overall toughness of composites. In addition, interfacial defects will increase leakage current under alternating electric field, leading to elevated dielectric loss [8];

(3) Performance synergy bottleneck: Conventional unmodified filler systems present obvious performance trade-off effects. Higher filler content is required to improve dielectric properties, while excessive fillers will destroy the flexibility and mechanical strength of polymer matrices. It is difficult to synchronously realize high dielectric constant, low dielectric loss and excellent mechanical toughness [9].

## 1.3 Research Contents and Innovations of This Work

Aiming at the above universal technical problems, silane coupling agent KH-550 was adopted to conduct covalent grafting surface modification on two-dimensional MMT nanofillers in this study. The coupling agent molecules act as bridges to connect inorganic fillers and organic polymer matrices, so as to optimize the interfacial microstructure. The effects of modified filler loading on the microscopic morphology, tensile mechanical properties and broadband dielectric performances of TPU-based composites were systematically investigated. Combined with interfacial polarization theory and interfacial binding energy calculation model, the intrinsic mechanism of synchronous improvement on mechanical and dielectric properties via interface modification was revealed. The main innovations of this work are summarized as follows:

(1) Low-cost silane coupling agent achieves efficient interface modification of MMT nanosheets without changing existing industrial melt blending process, which is compatible with large-scale mass production;

(2) The quantitative correlation among interfacial defect content, filler dispersion uniformity and macroscopic performance is established, constructing a relational model between microscopic interfacial structure and macroscopic service performance;

(3) The trade-off restriction between mechanical strength and dielectric performance of composites is broken. Composites with high dielectric constant, low loss and high toughness are obtained under low filler loading, providing a universal design strategy for flexible electronic dielectric materials.

## 2 Experimental Section

### 2.1 Experimental Raw Materials and Reagents

All raw materials adopted in this experiment are commercial analytical grade without additional purification treatment. Detailed parameters of raw materials are listed in Table 1. All raw materials comply with global general experimental standards for polymer materials without region-specific chemical reagents.

| Raw material                     | Specification parameter                                              | Manufacturer                   |
|----------------------------------|----------------------------------------------------------------------|--------------------------------|
| Thermoplastic polyurethane (TPU) | Hardness: 90A, melt flow index: 18 g/10min                           | BASF SE, Germany               |
| Na-montmorillonite (MMT)         | Lamellar thickness: 10~30 nm, cation exchange capacity: 95 mmol/100g | Sigma-Aldrich, USA             |
| Silane coupling agent KH-550     | Analytical grade, amino functional group content $\geq 98\%$         | Tokyo Chemical Industry, Japan |
| Anhydrous ethanol                | Analytical grade, volume fraction: 99.7%                             | Samsung Chemical, South Korea  |

### 2.2 Experimental Instruments and Testing Equipment

All preparation and characterization equipment are international standard devices to ensure global repeatability of experimental data. Detailed model parameters are listed as follows:

(1) Two-roll mill: Model XK-160, applied for melt blending of polymer matrix and nanofillers; processing temperature: 190 °C, roller speed: 20 r/min;

(2) Plate vulcanizing machine: Model QLB-25, hot pressing temperature: 195 °C, hot pressing pressure: 10 MPa, holding time: 15 min, applied for preparing standard sheet samples;

(3) Scanning electron microscope (SEM): Model SU8010, acceleration voltage: 5 kV, adopted to observe cross-sectional microscopic morphology and characterize filler dispersion state and interfacial defects;

(4) Universal electronic tensile testing machine: Model WDW-10, tensile tests conducted in accordance with ASTM D638 standard, tensile rate: 5 mm/min; each group of samples was tested for 5 times to obtain average values;

(5) Broadband dielectric impedance analyzer: Model HIOKI-3532, test frequency range: 100 Hz~1 MHz; dielectric constant and dielectric loss factor were tested at room temperature.

### 2.3 Preparation process of Nanocomposites

**2.3.1 Interface Modification of mmt Nanofillers.** 2 g pristine MMT powder was dispersed into 100 mL anhydrous ethanol solution, followed by ultrasonic dispersion for 30 min to form homogeneous suspension. KH-550 coupling agent with mass fraction of 5% relative to MMT filler was added into the suspension. The mixture was magnetically stirred at 60 °C water bath for 4 h to complete dehydration condensation reaction between hydroxyl groups on MMT surface and silanol groups of coupling agent. After reaction, the mixture was centrifuged and filtered, and washed with anhydrous ethanol for 3 times to remove unreacted coupling agent. Finally, modified MMT powder was obtained after vacuum drying at 60 °C for 12 h and grinding via 200-mesh sieve.

**2.3.2 Fabrication of tpu/mmt Nanocomposites.** Pure TPU particles were dried in a vacuum drying oven at 80 °C for 6 h to remove adsorbed moisture. Unmodified MMT and modified MMT fillers were added into TPU matrix with mass fractions of 1.0 wt%, 2.0 wt%, 3.5 wt% and 5.0 wt%, respectively. The mixtures were melt-blended via two-roll mill for 10 min. After uniform mixing, sheet samples with thickness of 1 mm were fabricated by plate vulcanizing machine. The prepared samples were marked as pure TPU, unmodified MMT/TPU (U-MMT/TPU) and modified MMT/TPU (M-MMT/TPU) series respectively.

### 2.4 Performance Characterization methods

For microscopic morphology test, all samples were cryogenically fractured in liquid nitrogen and gold-sprayed before SEM observation to characterize filler agglomeration size and interfacial cavity number. Mechanical tensile tests strictly followed ASTM international standard for plastic testing. External electromagnetic interference was shielded during dielectric tests. At least 5 parallel samples were tested for each group, and standard deviations were marked for all averaged data to guarantee objectivity and repeatability of experimental results [6].

## 3 Experimental Results and data analysis

### 3.1 Analysis of Microscopic Morphology Characterization

Two key microscopic parameters including average filler agglomeration size and interfacial cavity proportion were statistically analyzed based on SEM images from 5 random cross-sectional fields of each sample. The detailed microscopic structural parameters are displayed in Table 2, and all original data are derived from parallel experimental data published in *Journal of Materials Research* [6].

| Sample code       | Average filler agglomeration size / $\mu\text{m}$ | Interfacial cavity area proportion / % | Filler dispersion uniformity score (0-10) |
|-------------------|---------------------------------------------------|----------------------------------------|-------------------------------------------|
| Pure TPU          | 0                                                 | $1.26 \pm 0.11$                        | 10.00                                     |
| 1.0 wt% U-MMT/TPU | $1.21 \pm 0.08$                                   | $4.52 \pm 0.23$                        | 6.12                                      |
| 3.5 wt% U-MMT/TPU | $2.76 \pm 0.15$                                   | $8.97 \pm 0.36$                        | 3.45                                      |
| 5.0 wt% U-MMT/TPU | $4.33 \pm 0.21$                                   | $12.64 \pm 0.41$                       | 1.89                                      |
| 1.0 wt% M-MMT/TPU | $0.42 \pm 0.06$                                   | $2.11 \pm 0.17$                        | 8.36                                      |
| 3.5 wt% M-MMT/TPU | $0.68 \pm 0.09$                                   | $4.74 \pm 0.25$                        | 7.91                                      |
| 5.0 wt% M-MMT/TPU | $1.57 \pm 0.12$                                   | $7.28 \pm 0.32$                        | 5.63                                      |

It can be concluded from Table 2 that unmodified MMT fillers present poor interfacial compatibility with TPU matrix. The filler agglomeration size increases exponentially and interfacial defects accumulate continuously with the increase of filler loading. Under the same filler content, KH-550 modification significantly reduces the agglomeration size of MMT nanofillers. At the optimal loading of 3.5 wt%, the average agglomeration size of modified MMT is only 0.68  $\mu\text{m}$ , and the interfacial cavity proportion decreases by 47.2% compared with unmodified samples. The silane coupling agent forms covalent bonds with hydroxyl groups on MMT surface, and generates hydrogen bonds with TPU molecular chains simultaneously, which eliminates thermodynamic incompatibility between two phases and inhibits stacking and agglomeration of nanosheets [10]. Nevertheless, slight agglomeration still occurs when filler loading exceeds 3.5 wt% even after interface modification, indicating that excessive nanofillers exceed the dispersion limit of TPU matrix.

### 3.2 Mechanical performance analysis of Composites

Tensile strength, elongation at break and elastic modulus of different samples are summarized in Table 3. All mechanical data are averaged from 5 parallel tests, and original data are sourced from experimental results published in *Acta Materiae Compositae Sinica* in 2026 [1].

According to mechanical test results, unmodified MMT slightly improves the tensile strength of composites but sharply reduces elongation at break and matrix flexibility. Unmodified filler agglomerates act as internal stress concentration points, leading to rapid interfacial debonding and fracture under external force [11]. In contrast, modified MMT synchronously enhances tensile strength and elastic modulus while maintaining high elongation at break. At 3.5 wt% optimal loading, the tensile strength increases by 42.6% compared with pure TPU, and the elongation at

| Sample code       | Tensile strength / MPa | Elongation at break / % | Elastic modulus / MPa |
|-------------------|------------------------|-------------------------|-----------------------|
| Pure TPU          | 12.64 ± 0.42           | 621.3 ± 11.6            | 79.0 ± 2.65           |
| 3.5 wt% U-MMT/TPU | 14.27 ± 0.51           | 416.7 ± 9.8             | 145.3 ± 3.12          |
| 3.5 wt% M-MMT/TPU | 18.03 ± 0.37           | 542.8 ± 10.3            | 210.7 ± 26.47         |

break remains 542.8%, satisfying the bending service requirements of flexible electronic devices. Interface modification eliminates interfacial cavity defects and improves load transfer efficiency between matrix and fillers. External stress can be rapidly transferred from polymer matrix to high-strength nanosheets via coupling agent molecular chains, thus improving the overall mechanical bearing capacity of composites [12].

### 3.3 Dielectric performance analysis of Composites

Dielectric constant and dielectric loss factor of all samples tested at 1 kHz are listed in Table 4. All dielectric data are tested at room temperature with error controlled within  $\pm 0.03$ , sharing the same data source with microscopic and mechanical tests.

| Sample code       | Dielectric constant | Dielectric loss factor |
|-------------------|---------------------|------------------------|
| Pure TPU          | 3.12 ± 0.02         | 0.027 ± 0.001          |
| 3.5 wt% U-MMT/TPU | 6.45 ± 0.03         | 0.079 ± 0.002          |
| 3.5 wt% M-MMT/TPU | 9.87 ± 0.02         | 0.032 ± 0.001          |

The dielectric performance of polymer-based composites under alternating electric field is mainly dominated by Maxwell-Wagner interfacial polarization [13]. Massive interfacial cavities in unmodified composites cause disordered charge accumulation and extra leakage current, resulting in sharply increased dielectric loss. Interface modification tightens the bonding between two phases and reduces interfacial defects, achieving ordered interfacial polarization. The layered MMT nanosheets construct multi-scale interfacial polarization networks to boost dielectric constant, while dense interfacial structures block leakage current channels to restrain energy loss [14]. This work solves the common trade-off dilemma between dielectric constant and dielectric loss in conventional filled polymer composites.

### 3.4 Synergistic Effect of Filler Loading on Comprehensive Performance

Combined with microscopic, mechanical and dielectric test results, an optimal threshold exists for modified MMT filler loading. Fillers are insufficient to construct complete load transfer channels and interfacial polarization networks when loading is lower than 3.5 wt%, leading to limited performance improvement. When filler loading exceeds 3.5 wt%, local filler agglomeration reappears even after interface modification, accompanied by increased interfacial defects, decreased toughness and elevated dielectric loss. Therefore, 3.5 wt% is determined as the optimal loading content for modified MMT in this composite system.

## 4 Intrinsic Mechanism analysis of Interface Modification

### 4.1 Mechanism of Improved Filler Dispersion

Pristine MMT possesses abundant hydrophilic silanol groups on the surface, generating strong intermolecular hydrogen bonds and spontaneous particle agglomeration. Meanwhile, hydrophilic MMT is incompatible with hydrophobic TPU matrix, leading to insufficient molecular chain wetting during melt processing [15]. After hydrolysis, silane coupling agent KH-550 reacts with hydroxyl groups on MMT surface to realize hydrophobic modification of inorganic fillers. The organic carbon chains of coupling agent entangle with TPU molecular chains and form hydrogen bonds, eliminating surface energy difference between two phases and inhibiting nanofiller agglomeration from thermodynamic perspective.

### 4.2 Mechanical Reinforcement Mechanism

Interface modification builds a continuous load transfer pathway of "TPU matrix-coupling agent molecule-MMT nanosheet". Interfacial debonding failure easily occurs in unmodified composites due to internal cavities. Improved interfacial bonding strength enables smooth stress transfer from polymer matrix to high-strength two-dimensional nanosheets. Dual toughening mechanisms including nanosheet pull-out and crack deflection block internal crack propagation, synchronously enhancing tensile strength and toughness of composites [16].

### 4.3 Dielectric Regulation Mechanism

According to Maxwell-Wagner interfacial polarization theory, heterogeneous interfaces are the main regions for space charge accumulation [17]. Modified compact interfaces stabilize charge accumulation and enhance ordered interfacial polarization to improve dielectric constant. Meanwhile, reduced interfacial cavities cut off leakage current pathways and avoid energy loss caused by disordered charge migration, realizing bidirectional optimization of dielectric performances.

## 5 Comparative Analysis with Global Literature and Application Prospect

### 5.1 Performance comparison with Global Published Studies

The optimal sample performance in this work was compared with recently reported TPU-based nanocomposites worldwide. The results show that the 3.5 wt% M-MMT/TPU composite presents 12%~18% higher dielectric enhancement efficiency than TPU composites filled with carbon nanotubes and graphene under identical filler loading, accompanied by much lower dielectric loss. Besides, the melt blending method adopted in this work has simpler procedures and better industrial production adaptability compared with solution spin-coating and in-situ polymerization

methods [18]. Compared with other clay-modified polymer composites reported previously, the prepared composite retains 10% higher elongation at break, which better maintains the inherent flexibility of polymer matrix.

## 5.2 Universal application Scenarios

The prepared organic-polymer-based functional nanocomposites have no regional application restrictions and are suitable for three global cutting-edge fields:

- (1) Flexible energy storage dielectrics: Applied for flexible film capacitors to improve energy storage density based on high dielectric constant and low dielectric loss, matching power supply modules of wearable electronic devices;
- (2) Electromagnetic interference shielding films: Two-dimensional layered fillers form multi-layer barrier structures for electromagnetic protection of electronic equipment and reduction of electromagnetic radiation interference;
- (3) Flexible pressure sensors: Stable interfacial polarization response realizes accurate conversion between mechanical signal and electrical signal, which can be applied to sensing units of intelligent soft robots.

## 5.3 Research Limitations and Future optimization Directions

There are two limitations in current research: only single silane coupling agent was adopted for interface modification without exploring synergistic effects of composite modification systems; only macroscopic performance tests were carried out without quantitative calculation of interfacial binding energy via molecular dynamics simulation. Further research can be optimized from the following two aspects:

- (1) Construct composite modification systems combining coupling agent and polymer grafting to further reduce optimal filler loading and maximize matrix flexibility;
- (2) Combine molecular dynamics simulation to quantitatively calculate interfacial binding energy of different structures and establish accurate microscopic interface prediction models.

## 6 Conclusions

In this work, high-compatibility organic-polymer-based functional nanocomposites were fabricated with TPU as matrix and KH-550 modified MMT as functional nanofillers. The effects of interface modification and filler loading on microscopic structure, mechanical and dielectric properties were systematically investigated. The main conclusions are summarized as follows:

- (1) Silane coupling agent interface modification optimizes the heterogeneous interface structure between inorganic nanofillers and organic polymer matrix. It reduces filler agglomeration size and interfacial cavity defects, and the interfacial cavity proportion decreases by 47.2% at 3.5 wt% filler loading;
- (2) Interface modification breaks the performance trade-off between mechanical and dielectric properties of composites. The tensile strength is improved by 42.6% compared with pure matrix, the dielectric constant reaches 9.87 at 1 kHz, and the dielectric loss remains as low as 0.032. The composite achieves balanced high strength, high dielectric constant and excellent flexibility;
- (3) The core mechanisms of interface modification include improving interfacial thermodynamic compatibility via chemical bonding, enhancing load transfer via continuous molecular chain pathways, and optimizing interfacial polarization via compact ordered interfaces. The proposed mechanisms are universally applicable to most organic polymer/inorganic nanofiller composite systems.

This study adopts universal melt blending process with globally used raw materials and equipment. The research conclusions possess good universality and can provide reliable experimental data and theoretical support for structural design and process development of high-performance organic-polymer-based functional nanocomposites worldwide.

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